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One- and two-dimensional Coulomb Green's function matrices in parabolic Sturmians basis

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Abstract

One- and two-dimensional operators which originate from the asymptotic form of the three-body Coulomb wave equation in parabolic coordinates are treated within the context of a square integrable basis set. The matrix representations of Green's functions corresponding to these operators are obtained.

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1. Introduction

The three Coulomb (3C) wavefunctions [1, 2] have been introduced to approximate the three-body continuum Coulomb wave function. The 3C wave functions, provide asymptotics for the three-body wave functions in the region where the distances between the particles are large, but are not physically acceptable when the particles are near to each other. In the past few years many works have been published with different proposals to simply improve the 3C (see [3–5] and references therein). In this paper we seek to consider the possibilities for computing the three-body continuum Coulomb wavefunction which are afforded by expansion in a set of square-integrable functions. For the purpose of clarity, we outline the derivation [6] of the 3C wave functions.

The Hamiltonian of a three-body Coulomb system reads

$$H = \frac{1}{2\mu_{12}}\mathbf{K}^2 + \frac{1}{2\mu_3}\mathbf{k}^2 + \frac{Z_1Z_2}{r_{12}} + \frac{Z_2Z_3}{r_{23}} + \frac{Z_1Z_3}{r_{13}}. \tag{1}$$

Here, $\mathbf{K}$ and $\mathbf{k}$ are the momenta conjugate to the Jacobi vectors $\mathbf{R}$ and $\mathbf{r}$:

$$\mathbf{R} = \mathbf{r}_1 - \mathbf{r}_2, \qquad \mathbf{r} = \mathbf{r}_3 - \frac{m_1\mathbf{r}_1 + m_2\mathbf{r}_2}{m_1 + m_2}. \tag{2}$$

The reduced masses are

$$\mu_{12} = \frac{m_1m_2}{m_1 + m_2}, \qquad \mu_3 = \frac{(m_1 + m_2)m_3}{m_1 + m_2 + m_3}. \tag{3}$$

Inserting

$$\Psi = \mathrm{e}^{\mathrm{i}(\mathbf{K}\cdot\mathbf{R}+\mathbf{k}\cdot\mathbf{r})}\overline{\Psi} \tag{4}$$

into the Schrödinger equation

$$H\Psi = E\Psi\left(E = \frac{1}{2\mu_{12}}\mathbf{K}^2 + \frac{1}{2\mu_3}\mathbf{k}^2\right) \tag{5}$$

then yields

$$\mathrm{e}^{\mathrm{i}(\mathbf{K}\cdot\mathbf{R}+\mathbf{k}\cdot\mathbf{r})}\left[-\frac{1}{2\mu_{12}}\triangle_{\mathbf{R}} - \frac{1}{2\mu_3}\triangle_{\mathbf{r}} - \frac{\mathrm{i}}{\mu_{12}}\mathbf{K}\cdot\nabla_{\mathbf{R}} - \frac{\mathrm{i}}{\mu_3}\mathbf{k}\cdot\nabla_{\mathbf{r}} + \frac{Z_1Z_2}{r_{12}} + \frac{Z_2Z_3}{r_{23}} + \frac{Z_1Z_3}{r_{13}} + \frac{1}{2\mu_{12}}\mathbf{K}^2 + \frac{1}{2\mu_3}\mathbf{k}^2\right]\overline{\Psi} = \mathrm{e}^{\mathrm{i}(\mathbf{K}\cdot\mathbf{R}+\mathbf{k}\cdot\mathbf{r})}E\overline{\Psi}, \tag{6}$$

i.e.

$$\left[-\frac{1}{2\mu_{12}}\triangle_{\mathbf{R}} - \frac{1}{2\mu_3}\triangle_{\mathbf{r}} - \frac{\mathrm{i}}{\mu_{12}}\mathbf{K}\cdot\nabla_{\mathbf{R}} - \frac{\mathrm{i}}{\mu_3}\mathbf{k}\cdot\nabla_{\mathbf{r}} + \frac{Z_1Z_2}{r_{12}} + \frac{Z_2Z_3}{r_{23}} + \frac{Z_1Z_3}{r_{13}}\right]\overline{\Psi} = 0. \tag{7}$$

The differential operator

$$D = \frac{1}{2\mu_{12}}\triangle_{\mathbf{R}} + \frac{1}{2\mu_3}\triangle_{\mathbf{r}} + \frac{\mathrm{i}}{\mu_{12}}\mathbf{K}\cdot\nabla_{\mathbf{R}} + \frac{\mathrm{i}}{\mu_3}\mathbf{k}\cdot\nabla_{\mathbf{r}} \tag{8}$$

is considered in terms of parabolic coordinates introduced by Klar [6]

$$\xi_j = r_{ls} + \hat{\mathbf{k}}_{ls}\cdot\mathbf{r}_{ls}, \qquad \eta_j = r_{ls} - \hat{\mathbf{k}}_{ls}\cdot\mathbf{r}_{ls}, \tag{9}$$

where $\mathbf{r}_{ls}$ and $\mathbf{k}_{ls}$ are the relative coordinate and momentum vectors between the particles l and s. Here j, l, s is a cyclic permutation of 1, 2, 3. Klar [6] proposed to split D into two parts

$$D = D_0 + D_1. \tag{10}$$

The D_0 term contains one-variable derivatives $\frac{\partial}{\partial\xi_j}, \frac{\partial}{\partial\eta_j}, \frac{\partial^2}{\partial\xi_j^2}, \frac{\partial^2}{\partial\eta_j^2}$ whereas D_1 contains all mixed second derivatives $\frac{\partial^2}{\partial\xi_j\partial\xi_l}, \frac{\partial^2}{\partial\eta_j\partial\eta_l}, j \neq l$ and $\frac{\partial^2}{\partial\xi_j\partial\eta_l}$. Thus the D_0 term and Coulomb interactions form a leading term which provides a three-body continuum wavefunction that satisfies the exact asymptotic boundary conditions for Coulomb systems in the limit of all particles being far from each other. The operator D_1 is regarded as a small perturbation which does not violate the boundary conditions [6]. Then the approximate equation

$$\left[-D_0 + \frac{Z_1Z_2}{r_{12}} + \frac{Z_2Z_3}{r_{23}} + \frac{Z_1Z_3}{r_{13}}\right]\overline{\Psi} = 0 \tag{11}$$

in terms of parabolic coordinates (9) reads

$$\left\{\sum_{j=1}^{3}\frac{1}{\mu_{ls}(\xi_j+\eta_j)}[\hat{h}_{\xi_j} + \hat{h}_{\eta_j} + 2k_{ls}t_{ls}]\right\}\overline{\Psi} = 0, \tag{12}$$

where $t_{ls} = \frac{Z_lZ_s\mu_{ls}}{k_{ls}}$, $\mu_{ls} = \frac{m_lm_s}{m_l+m_s}$. Here the operators $\hat{h}_{\xi_j}$ and $\hat{h}_{\eta_j}$ are defined by

$$\begin{aligned}\hat{h}_{\xi_j} &= -2\left(\frac{\partial}{\partial\xi_j}\xi_j\frac{\partial}{\partial\xi_j} + \mathrm{i}k_{ls}\xi_j\frac{\partial}{\partial\xi_j}\right),\\ \hat{h}_{\eta_j} &= -2\left(\frac{\partial}{\partial\eta_j}\eta_j\frac{\partial}{\partial\eta_j} - \mathrm{i}k_{ls}\eta_j\frac{\partial}{\partial\eta_j}\right).\end{aligned} \tag{13}$$

Equation (12) is separable with infinite number of solutions. The solution $\overline{\Psi}$ can be represented in product form: [6]

$$\overline{\Psi} = \prod_{j=1}^{3} f_j(\xi_j, \eta_j) \tag{14}$$

and each of the functions $f_j(\xi_j, \eta_j)$ is a solution of equation [6]

$$\frac{1}{\mu_{ls}(\xi_j + \eta_j)}\left[\hat{h}_{\xi_j} + \hat{h}_{\eta_j} + 2k_{ls}t_{ls}\right] f_j(\xi_j, \eta_j) = -C_j f_j(\xi_j, \eta_j). \tag{15}$$

The separation constants C_j have to satisfy the constraint [6]

$$C_1 + C_2 + C_3 = 0. \tag{16}$$

Equation (15) is again separable; therefore the solution can be represented in the form $f_j(\xi_j, \eta_j) = u_j(\xi_j)v_j(\eta_j)$. $u_j(\xi_j)$ and $v_j(\eta_j)$ satisfy the equations [6]

$$\begin{aligned} &\left[\hat{h}_{\xi_j} + 2k_{ls}A_j + \mu_{ls}C\xi_j\right]u_j(\xi_j) = 0, \\ &\left[\hat{h}_{\eta_j} + 2k_{ls}B_j + \mu_{ls}C\eta_j\right]v_j(\eta_j) = 0, \end{aligned} \tag{17}$$

where the separation constants A_j and B_j satisfy the constraint

$$A_j + B_j = t_{ls}. \tag{18}$$

The separation constants must have the values $C_j = B_j = 0$ and $A_j = t_{ls}$ for outgoing waves (coordinate ξ_j) or $C_j = A_j = 0$ and $B_j = t_{ls}$ for incoming waves (coordinate η_j) [3]. Regular solutions to (17) are [6]

$$u_j(\xi_j) = {}_1F_1(\mathrm{i}tls, 1; -\mathrm{i}k_{ls}\xi_j) \qquad (v_j(\eta_j) = 1 \text{ and } f_j(\xi_j, \eta_j) = u_j(\xi_j)) \tag{19}$$

for an outgoing wave, and

$$v_j(\eta_j) = {}_1F_1(-\mathrm{i}tls, 1; \mathrm{i}k_{ls}\eta_j) \qquad (u_j(\xi_j) = 1 \text{ and } f_j(\xi_j, \eta_j) = v_j(\eta_j)) \tag{20}$$

for an incoming wave. Thus a solution $\overline{\Psi}$ with pure outgoing behavior can be written as a product the of three independent two-body Coulomb wave functions:

$$\Psi_{3C} = \prod_{j=1}^{3} u_j(\xi_j). \tag{21}$$

2. Formulation of the problem

One way to improve Ψ_{3C} is to take into account (some terms of) D_1 that is expected to describe short-range Coulomb correlations [6]. We propose to expand the wavefunction $\overline{\Psi}$ in a square-integrable function series

$$\overline{\Psi} = \sum_{\mathcal{N}} a_{\mathcal{N}} |\mathcal{N}\rangle, \tag{22}$$

$$|\mathcal{N}\rangle = \prod_{j=1}^{3} \phi_{n_j m_j}(\xi_j, \eta_j). \tag{23}$$

The parabolic Sturmian functions $\phi_{n_j m_j}$ are used in (22) and (23),

$$\phi_{n_j m_j}(\xi_j, \eta_j) = \varphi_{n_j}(\xi_j)\varphi_{m_j}(\eta_j), \tag{24}$$

$$\varphi_n(x) = \sqrt{2b}\,\mathrm{e}^{-bx} L_n(2bx), \tag{25}$$

where b is the scale parameter. The summation in (22) is over n_j and m_j from 0 to ∞. The basis set (25) has been used in the analysis of the Coulomb potential within the parabolic formulation of the J-matrix method [10].

Let $\hat{\mathfrak{h}}$ denote the (long-range) operator which is obtained by multiplying the expression in the figured brackets on the left-hand side of (12) by $\prod_{j=1}^{3} \mu_{ls}(\xi_j + \eta_j)$ (from left). The (short-range) operator $\hat{V}$ is obtained by taking the product of $\prod_{j=1}^{3} \mu_{ls}(\xi_j + \eta_j)$ and the part of D_1 that is taken into account.The projection of the equation

$$[\hat{\mathfrak{h}} + \hat{V}]\overline{\Psi} = 0 \tag{26}$$

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

$$[\underline{\mathfrak{h}} + \underline{V}]\underline{a} = \mathbf{0}, \tag{27}$$

where $\underline{\mathfrak{h}}$ and $\underline{V}$ are the matrices with elements $\langle\mathcal{N}|\hat{\mathfrak{h}}|\mathcal{N}'\rangle$ and $\langle\mathcal{N}|\hat{V}|\mathcal{N}'\rangle$, respectively, and $\underline{a}$ is the vector with components $a_{\mathcal{N}}$. This equation can be rewritten, in view of the boundary condition (21), in the form

$$\underline{a} = \underline{a}^{(0)} - \underline{\mathfrak{h}}^{-1}\underline{V}\,\underline{a}, \tag{28}$$

where $a_{\mathcal{N}}^{(0)} = \langle\mathcal{N}|\Psi_{3C}\rangle$.

It is suggested that the short-range operator $\hat{V}$ can be approximated by a finite-order matrix $\underline{V}$. The operator $\hat{\mathfrak{h}}$ matrix $\underline{\mathfrak{h}}$ is infinite. Because of this, the six-dimensional resolvent operator matrix $\underline{\mathfrak{G}}$ (that is the matrix inverse of $\underline{\mathfrak{h}}$) should as far as possible be carried out analytically. This is a complicated problem. Note that $\hat{\mathfrak{h}}$ can be written, in view of (12), (15) and (16), as

$$\hat{\mathfrak{h}} = \mu_{13}(\xi_2+\eta_2)\mu_{12}(\xi_3+\eta_3)\hat{\mathfrak{h}}_1 + \mu_{23}(\xi_1+\eta_1)\mu_{12}(\xi_3+\eta_3)\hat{\mathfrak{h}}_2 + \mu_{23}(\xi_1+\eta_1)\mu_{13}(\xi_2+\eta_2)\hat{\mathfrak{h}}_3, \tag{29}$$

where

$$\hat{\mathfrak{h}}_j = \hat{h}_{\xi_j} + \hat{h}_{\eta_j} + 2k_{ls}t_{ls} + \mu_{ls}C_j(\xi_j+\eta_j). \tag{30}$$

In this paper we restrict ourselves to the construction of matrices of the Green' functions corresponding to the two-dimensional operators (30). First we consider the one-dimensional operators

$$\hat{h}_\xi + 2kt + C\xi, \qquad \hat{h}_\eta + 2k(t_0 - t) + C\eta \tag{31}$$

(Here we omit the indices and the factor μ_{ls}, the constraint (18) is also taken into account.) To treat these operators within the context of square-integrable basis set, the J-matrix method [7, 8] or the tools of the 'Tridiagonal Physics' program (see [9] and the reference therein) can be employed.

In section 3 using the tridiagonal matrix representations of one-dimensional operators (31) in the bases (25), we construct the corresponding Green's function matrices. In this case we do not seek to determine Green's matrices uniquely. In section 4 the weight function is obtained for the orthogonal polynomials satisfying the three-term recurrence relation. The two-dimensional Green's function matrix elements are expressed as convolution of one-dimensional Green's matrix elements in section 5. An orthogonality relation employed in the two-dimensional Green's matrix construction is derived in appendix.

3. One-dimensional Coulomb Green's function matrices

(a) $C = 0$

The matrix representation $\mathbf{h}_\xi + 2kt\mathbf{I}_\xi$ ($\mathbf{I}_\xi$ is the unit matrix) of the operator $\hat{h}_\xi + 2kt$ in the basis set $\{\varphi_n(\xi)\}_{n=0}^{\infty}$ (25) is tridiagonal:

$$\mathbf{h}_\xi + 2kt\mathbf{I}_\xi = \begin{pmatrix} b_0 & d_1 & & & \\ a_1 & b_1 & d_2 & & 0 \\ & a_2 & b_2 & d_3 & \\ & & a_3 & \times & \times \\ & 0 & & \times & \times & \times \end{pmatrix}, \tag{32}$$

where

$$b_n = (b + \mathrm{i}k) + 2bn + 2kt, \qquad a_n = (b - \mathrm{i}k)n, \qquad d_n = (b + \mathrm{i}k)n. \tag{33}$$

To construct the Green's function matrix $\mathbf{g}_\xi$, which is matrix inverse of the infinite tridiagonal matrix (32), consider the three-term recurrence relation

$$a_n w_{n-1} + b_n w_n + d_{n+1} w_{n+1} = 0, \qquad n \geqslant 1. \tag{34}$$

It can be easily verified that

$$p_n(t;\zeta) = \frac{(-1)^n}{n!}\frac{\Gamma(n+1-\mathrm{i}t)}{\Gamma(1-\mathrm{i}t)}\,{}_2F_1(-n, \mathrm{i}t; -n+\mathrm{i}t; \zeta), \tag{35}$$

where $\zeta = \frac{b-\mathrm{i}k}{b+\mathrm{i}k}$, is the 'regular' solution of (34) which satisfies the initial conditions:

$$p_0(t;\zeta) = 1, \qquad b_0 p_0(t;\zeta) + d_1 p_1(t;\zeta) = 0. \tag{36}$$

Suffice to say that apart from the factor $\sqrt{\frac{2}{b}}\left(\frac{\zeta+1}{2}\right)^{\mathrm{i}t}$, p_n is the coefficient of the nth basis function $\varphi_n(\xi)$ (25) in the expansion of $u(\xi)$ (19). Note that p_n are polynomials of degree n in t.

The second solution q_n of the recursion (34) can be obtained from the condition that q_n satisfies the same differential equation as p_n [8]. In other words, if $p_n \sim {}_2F_1(a, b; c; z)$, then $q_n \sim z^{1-c}{}_2F_1(a-c+1, b-c+1; 2-c; z)$. It is readily verified that an appropriate $q_n(t;\zeta)$ is

$$\begin{aligned} q_n(t;\zeta) &= -\frac{n!\Gamma(1-\mathrm{i}t)}{\Gamma(n+2-\mathrm{i}t)}(-\zeta)^{n+1}{}_2F_1(1-\mathrm{i}t, n+1; n+2-\mathrm{i}t; \zeta) \\ &= -\frac{n!\Gamma(1-\mathrm{i}t)}{\Gamma(n+2-\mathrm{i}t)}\left(\frac{\zeta}{\zeta-1}\right)^{n+1}{}_2F_1\left(n+1, n+1; n+2-\mathrm{i}t; \frac{\zeta}{\zeta-1}\right). \end{aligned} \tag{37}$$

This satisfies the initial condition

$$b_0 q_0(t;\zeta) + d_1 q_1(t;\zeta) = b - \mathrm{i}k. \tag{38}$$

Multiplying $[\mathbf{h}_\xi + 2kt\mathbf{I}_\xi]$ by the diagonal matrix $\mathbf{Z} = [1, \zeta^{-1}, \ldots, \zeta^{-n}, \ldots]$, we obtain the symmetric tridiagonal matrix $\mathbf{T}$:

$$\mathbf{T} = \mathbf{Z}[\mathbf{h}_\xi + 2kt\mathbf{I}_\xi] = \begin{pmatrix} \beta_0 & \alpha_1 & & & \\ \alpha_1 & \beta_1 & \alpha_2 & & 0 \\ & \alpha_2 & \beta_2 & \alpha_3 & \\ & & \alpha_3 & \times & \times \\ & 0 & & \times & \times & \times \end{pmatrix} \tag{39}$$

with nonzero elements

$$\beta_n = b_n/\zeta^n, \qquad \alpha_n = d_n/\zeta^{n-1}. \tag{40}$$

Note that p_n and q_n satisfy the three-term recurrence relation

$$\alpha_n w_{n-1} + \beta_n w_n + \alpha_{n+1} w_{n+1} = 0, \qquad n \geqslant 1. \tag{41}$$

Thus, to invert the symmetric tridiagonal matrix $\mathbf{T}$, one can draw on the standard method [11, 12]. Namely, the elements of a Green's matrix $\mathbf{g}_T$, which is the matrix inverse to $\mathbf{T}$, can be determined by

$$g^T_{nm}(t) = \frac{p_\nu(t;\zeta)q_\mu(t;\zeta)}{W(q,p)}. \tag{42}$$

Henceforward μ and ν are the greater and lesser of n and m, respectively. The Wronskian W is defined as

$$\begin{aligned} W(q,p) &= \alpha_n[q_n(t;\zeta)p_{n-1}(t;\zeta) - q_{n-1}(t;\zeta)p_n(t;\zeta)] \\ &= b - \mathrm{i}k = -2\mathrm{i}k\left(\frac{\zeta}{\zeta-1}\right). \end{aligned} \tag{43}$$

Green's matrix $\mathbf{g}_\xi = [\mathbf{h}_\xi + 2kt\mathbf{I}_\xi]^{-1}$ is related to $\mathbf{g}_T$: $\mathbf{g}_\xi = \mathbf{g}_T\mathbf{Z}$. Therefore, we can express the matrix $\mathbf{g}_\xi$ elements in the form

$$g^\xi_{nm}(t) = \frac{\mathrm{i}}{2k}\left(\frac{\zeta-1}{\zeta}\right)\frac{1}{\zeta^m}p_\nu(t;\zeta)q_\mu(t;\zeta). \tag{44}$$

From (13) it follows that Green's matrix $\mathbf{g}_\eta = [\mathbf{h}_\eta + 2kt\mathbf{I}_\eta]^{-1}$ and $\mathbf{g}_\xi$ are complex conjugates (for real k and t):

$$g^\eta_{nm}(t) = \left(g^\xi_{nm}(t)\right)^*. \tag{45}$$

Note that there is an ambiguity in determining the matrix $\mathbf{g}_\xi$, since the solution $q_n(t;\zeta)$ is not unique:

$$\widetilde{q}_n(t;\zeta) = q_n(t;\zeta) + y(t)p_n(t;\zeta), \tag{46}$$

where $y(t)$ is an arbitrary function of t, also satisfies (34).

(b) $C \neq 0$

It is not difficult to convince oneself that the differential equation

$$[\hat{h}_\xi + 2kt + C\xi]u(\xi) = 0 \tag{47}$$

is satisfied by the function

$$u(\xi) = \mathrm{e}^{\frac{\mathrm{i}}{2}(\gamma-k)\xi}\,{}_1F_1(\mathrm{i}\tau, 1; -\mathrm{i}\gamma\xi), \tag{48}$$

where

$$\gamma = k\sqrt{1-\frac{2C}{k^2}}, \qquad \tau = \frac{k}{\gamma}\left(t+\frac{\mathrm{i}}{2}\right) - \frac{\mathrm{i}}{2}. \tag{49}$$

Clearly, in the limit $C = 0$ the function (48) reduces to (19).

Because the operator ξ, evaluated in the basis (25), has the symmetric tridiagonal form

$$Q_{n,n'} = \begin{cases} -\frac{1}{2b}n, & n' = n-1, \\ \frac{1}{2b}(2n+1), & n' = n, \\ -\frac{1}{2b}(n+1), & n' = n+1, \end{cases} \tag{50}$$

the matrix representation of the operator $\hat{h}_\xi + 2kt + C\xi$ is also tridiagonal. Thus,

$$\mathbf{h}_\xi + 2kt\mathbf{I}_\xi + C\mathbf{Q}_\xi = \begin{pmatrix} b_0 & d_1 & & & & \\ a_1 & b_1 & d_2 & & 0 & \\ & a_2 & b_2 & d_3 & & \\ & & a_3 & \times & \times & \\ & 0 & & \times & \times & \times \end{pmatrix}, \tag{51}$$

where

$$\begin{aligned} b_n &= \left(b + \frac{C}{2b} + \mathrm{i}k\right) + 2\left(b + \frac{C}{2b}\right) n + 2kt, \\ a_n &= \left(b - \frac{C}{2b} - \mathrm{i}k\right) n, \qquad d_n = \left(b - \frac{C}{2b} + \mathrm{i}k\right) n. \end{aligned} \tag{52}$$

Then, if we consider the coefficients of the regular solution (48) expansion in the basis set (25), we obtain that

$$s_n(t; C) = \theta^n p_n(\tau; \zeta), \tag{53}$$

where

$$\theta = \frac{2b + \mathrm{i}(\gamma - k)}{2b - \mathrm{i}(\gamma - k)}, \qquad \lambda = \frac{2b - \mathrm{i}(\gamma + k)}{2b + \mathrm{i}(\gamma + k)}, \qquad \zeta = \frac{\lambda}{\theta}, \tag{54}$$

is the solution of the three-term recurrence relation

$$a_n w_{n-1} + b_n w_n + d_{n+1} w_{n+1} = 0, \qquad n \geqslant 1. \tag{55}$$

It is easy to verify that two linearly independent second solutions of equation (55) can be expressed in the form

$$\begin{aligned} c_n^{(-)}(t; C) &= (-)^n \lambda^{n+1} \frac{n!\Gamma(1 - \mathrm{i}\tau)}{\Gamma(n + 2 - \mathrm{i}\tau)} {}_2F_1(1 - \mathrm{i}\tau, n + 1; n + 2 - \mathrm{i}\tau; \zeta), \\ c_n^{(+)}(t; C) &= (-)^n \theta^{n+1} \frac{n!\Gamma(\mathrm{i}\tau)}{\Gamma(n + 1 + \mathrm{i}\tau)} {}_2F_1(\mathrm{i}\tau, n + 1; n + 1 + \mathrm{i}\tau; \zeta^{-1}). \end{aligned} \tag{56}$$

Note that the matrix $\mathbf{h}_\xi + 2kt\mathbf{I}_\xi + C\mathbf{Q}_\xi$ inversion procedure is simplified if we introduce the symmetric tridiagonal matrix $\mathbf{T}$:

$$\mathbf{T} = \mathbf{Z}[\mathbf{h}_\xi + 2kt\mathbf{I}_\xi + C\mathbf{Q}_\xi] = \begin{pmatrix} \beta_0 & \alpha_1 & & & & \\ \alpha_1 & \beta_1 & \alpha_2 & & 0 & \\ & \alpha_2 & \beta_2 & \alpha_3 & & \\ & & \alpha_3 & \times & \times & \\ & 0 & & \times & \times & \times \end{pmatrix}. \tag{57}$$

Here $\mathbf{Z}$ is the diagonal matrix: $\mathbf{Z} = [1, \chi^{-1}, \ldots, \chi^{-n}, \ldots]$, $\chi = \frac{b - \frac{C}{2b} - \mathrm{i}k}{b - \frac{C}{2b} + \mathrm{i}k}$. The elements β_n and α_n are given by

$$\beta_n = b_n / \chi^n, \qquad \alpha_n = d_n / \chi^{n-1}. \tag{58}$$

Then, it is easy to check that s_n and c_n also satisfy the recursion equation

$$\alpha_n w_{n-1} + \beta_n w_n + \alpha_{n+1} w_{n+1} = 0, \qquad n \geqslant 1, \tag{59}$$

and the Wronskian

$$W(c^{(\pm)}, s) = \alpha_n \left[c_n^{(\pm)}(t; C) s_{n-1}(t; C) - c_{n-1}^{(\pm)}(t; C) s_n(t; C)\right] \tag{60}$$

is independent of n. Namely,

$$W(c^{(\pm)}, s) = b - \frac{C}{2b} - \mathrm{i}k = -2\mathrm{i}k\left(\frac{\chi}{\chi - 1}\right). \tag{61}$$

Finally, given the two linearly independent solutions s_n and $c_n^{(-)}$ of equation (55), we can express Green's matrix $\mathbf{g}_\xi = [\mathbf{h}_\xi + 2kt\mathbf{I}_\xi + C\mathbf{Q}_\xi]^{-1}$ elements in the form

$$g_{nm}^{\xi}(t; C) = \frac{s_\nu(t; C)c_\mu^{(-)}(t; C)}{W(c^{(-)}, s)}\chi^{-m} = \frac{\mathrm{i}}{2k}\left(\frac{\chi - 1}{\chi}\right)\frac{\theta^{n+m+1}}{\chi^m}p_\nu(\tau; \zeta)q_\mu(\tau; \zeta). \tag{62}$$

Clearly, Green's matrix $\mathbf{g}_\eta = [\mathbf{h}_\eta + 2kt\mathbf{I}_\eta + C\mathbf{Q}_\eta]^{-1}$ is obtained from $\mathbf{g}_\xi$ by replacing $t \to -t$, $k \to -k$ (this leaves kt unchanged).

4. Orthogonal polynomials p_n

In this section we obtain the weight function with respect to which the polynomials p_n (35) are orthonormal.

Kummer's relation (15.3.7) in [13] expresses the solution $c_n^{(+)}$ as a combination of the other two:

$$c_n^{(+)}(\tau; C) = c_n^{(-)}(\tau; C) + 2\pi\mathrm{i}\theta\rho(\tau; \zeta)s_n(\tau; C), \tag{63}$$

where

$$\rho(\tau; \zeta) = \frac{\Gamma(1 - \mathrm{i}\tau)\Gamma(\mathrm{i}\tau)}{2\pi\mathrm{i}}(-\zeta)^{\mathrm{i}\tau}. \tag{64}$$

Henceforward it is considered that

$$|\arg(-\zeta)| < \pi. \tag{65}$$

Consider the integral

$$\mathcal{I}(\zeta) = \int_{\mathcal{C}} \mathrm{d}\tau\rho(\tau; \zeta), \tag{66}$$

where $\mathcal{C}$ runs along the real axis, except for an infinitesimal indentation on the underside of the pole $\tau = 0$; see figure 1. By closing the contour in the upper half of the complex τ-plane $\mathcal{I}(\zeta)$ is reduced to the sum of the residues at the poles $\tau_\ell = \mathrm{i}\ell$, $\ell = 0, 1, \ldots, \infty$:

$$\mathcal{I}(\zeta) = -\mathrm{i}\sum_{\ell=0}^{\infty}\frac{1}{\zeta^\ell}, \tag{67}$$

i.e.

$$\mathcal{I}(\zeta) = \frac{\mathrm{i}\zeta}{1 - \zeta}. \tag{68}$$

Note that for $\mathrm{Im}(\zeta) \neq 0$ (65) implies that

$$\rho(\tau; \zeta) = \begin{cases} \dfrac{\zeta^{\mathrm{i}\tau}}{1 - \mathrm{e}^{2\pi\tau}}, & -\pi < \arg(\zeta) < 0, \\ \dfrac{\zeta^{\mathrm{i}\tau}}{\mathrm{e}^{-2\pi\tau} - 1}, & 0 < \arg(\zeta) < \pi. \end{cases} \tag{69}$$

Using the Sokhotsky formula we obtain

$$\mathcal{I}(\zeta) = \mathcal{P}\int_{-\infty}^{\infty} \mathrm{d}\tau\, \rho(\tau; \zeta) - \frac{\mathrm{i}}{2}. \tag{70}$$

In this case (69) provides the convergence of the principal-value integral on the right hand side of (70).

Clearly, integrals

$$\int_{\mathcal{C}} \mathrm{d}\tau \rho(\tau;\zeta) p_n(\tau;\zeta) p_m(\tau;\zeta) \tag{71}$$

can be expanded in terms of derivatives of (66). It is now easy to obtain that

$$\frac{\mathrm{i}}{\zeta^n}\left(\frac{\zeta-1}{\zeta}\right)\int_{\mathcal{C}} \mathrm{d}\tau \rho(\tau;\zeta) p_n(\tau;\zeta) p_m(\tau;\zeta) = \delta_{nm}, \tag{72}$$

i.e. ρ (64) is the weight function for the orthogonal polynomials p_n (35).

For $\mathrm{Im}(\zeta) \neq 0$ we can rewrite the orthonormality relation (72) as

$$\frac{\mathrm{i}}{\zeta^n}\left(\frac{\zeta-1}{\zeta}\right)\left(\mathcal{P}\int_{-\infty}^{\infty} \mathrm{d}\,\tau \rho(\tau;\zeta) p_n(\tau;\zeta) p_m(\tau;\zeta) - \frac{\mathrm{i}}{2}(-1)^{n+m}\right) = \delta_{nm}, \tag{73}$$

where the weight function ρ in the form of (69) is used. Note that in the case of $C = 0$ we have $\zeta = \mathrm{e}^{\mathrm{i}\varphi}$, $\varphi < 0$, and the weight function reduces to

$$\rho_0(t;\zeta) = \frac{\mathrm{e}^{-\varphi t}}{1-\mathrm{e}^{2\pi t}}. \tag{74}$$

It is preferable, however, to use the weight function

$$\sigma(s;\zeta) \equiv \rho\left(s - \frac{\mathrm{i}}{2};\zeta\right) = \frac{\Gamma\left(\frac{1}{2}-\mathrm{i}s\right)\Gamma\left(\frac{1}{2}+\mathrm{i}s\right)}{2\pi\mathrm{i}}(-\zeta)^{\mathrm{i}s+\frac{1}{2}}. \tag{75}$$

It is readily verified that

$$\int_{-\infty}^{\infty} \mathrm{d}s\,\sigma(s;\zeta) = \frac{\mathrm{i}\zeta}{1-\zeta} \tag{76}$$

and therefore

$$\frac{\mathrm{i}}{\zeta^n}\left(\frac{\zeta-1}{\zeta}\right)\int_{-\infty}^{\infty} \mathrm{d}s\,\sigma(s;\zeta) p_n\left(s-\frac{\mathrm{i}}{2};\zeta\right) p_m\left(s-\frac{\mathrm{i}}{2};\zeta\right) = \delta_{nm}. \tag{77}$$

It may be remarked that the polynomials p_n are discrete analogues of the charge parabolic Coulomb Sturmians introduced in [14].

5. Two-dimensional Green's function matrices

In this section we obtain a matrix representation $\mathbf{G}(t_0; C)$ of Green's function (resolvent) of the operator

$$\hat{\mathfrak{h}} = \hat{h}_\xi + \hat{h}_\eta + 2kt_0 + C(\xi+\eta). \tag{78}$$

Formally $\mathbf{G}(t_0; C)$ is the matrix inverse of the infinite matrix

$$\mathbf{h} = \mathbf{h}_\xi \otimes \mathbf{I}_\eta + \mathbf{I}_\xi \otimes \mathbf{h}_\eta + 2kt_0 \mathbf{I}_\xi \otimes \mathbf{I}_\eta + C(\mathbf{Q}_\xi \otimes \mathbf{I}_\eta + \mathbf{I}_\xi \otimes \mathbf{Q}_\eta), \tag{79}$$

i.e.

$$\mathbf{h}\mathbf{G}(t_0; C) = \mathbf{I}_\xi \otimes \mathbf{I}_\eta. \tag{80}$$

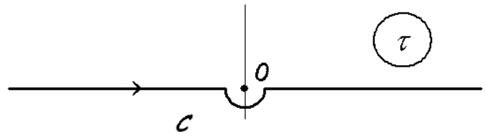

Figure 1. The path of integration $\mathcal{C}$ in (66).

(a) $C = 0$

The elements of $\mathbf{G}(t_0) \equiv \mathbf{G}(t_0; 0)$ can be expressed as a convolution integral (see, e.g. [15])

$$G_{n_1n_2,m_1m_2}(t_0) = \int_{\mathcal{C}_0} \mathrm{d}t\, \tilde{g}^{\xi}_{n_1m_1}(t)\tilde{g}^{\eta}_{n_2m_2}(t_0 - t), \tag{81}$$

where the integrand contains functions $\tilde{g}^{\xi}_{nm}$ and $\tilde{g}^{\eta}_{nm}$ that are proportional to the one-dimensional Green's function matrix elements (the non-uniqueness (46) of the solution q_n is taken into account):

$$\tilde{g}^{\xi}_{nm}(t) = \frac{\mathrm{i}}{2k}\left(\frac{\zeta - 1}{\zeta}\right)\frac{1}{\zeta^m} p_\nu(t;\zeta)[A_\xi q_\mu(t;\zeta) + x_\mu(t)p_\mu(t;\zeta)]B_m \tag{82}$$

and

$$\tilde{g}^{\eta}_{nm}(t) = \frac{\mathrm{i}}{2k}(\zeta - 1)\zeta^m p_\nu(-t;\zeta^{-1})[A_\eta q_\mu(-t;\zeta^{-1}) + y_\mu(t)p_\mu(-t;\zeta^{-1})]D_m. \tag{83}$$

Inserting (81)–(83) into (80) then gives the restriction on the factors A_ξ and A_η, functions $\{x_n(t)\}_{n=0}^{\infty}$ and $\{y_n(t)\}_{n=0}^{\infty}$, diagonal matrices $\mathbf{B} = [B_0, B_1, \ldots]$ and $\mathbf{D} = [D_0, D_1, \ldots]$, and the path of integration $\mathcal{C}_0$, namely,

$$A_\eta D_{m_2} \int_{\mathcal{C}_0} \mathrm{d}t\ \tilde{g}^{\xi}_{n_1m_1}(t) = U_{n_1m_2}\delta_{n_1m_1}, \tag{84}$$

$$A_\xi B_{m_1} \int_{\mathcal{C}_0} \mathrm{d}t\, \tilde{g}^{\eta}_{n_2m_2}(t_0 - t) = V_{m_1n_2}\delta_{n_2m_2}, \tag{85}$$

$$U_{n_1m_2} + V_{m_1n_2} = 1. \tag{86}$$

If we choose the contour $\mathcal{C}$ (see figure 1) as the path of integration in (81) (and (84), (85)), we can draw on the orthonormality relation (72) to determine the rest of the parameters. In this case we readily check that, in particular, the set: $A_\xi = 0, x_n(t) = 2\pi\mathrm{i}\rho_0(t;\zeta), A_\eta = \frac{k}{\mathrm{i}\pi}, y_n(t) \equiv 0, B_n = D_n = 1$, satisfies conditions (84)–(86), and hence the elements $G_{n_1n_2,m_1m_2}$ can be expressed in the form

$$G_{n_1n_2,m_1m_2}(t_0) = \frac{\mathrm{i}}{\zeta^{m_1}}\left(\frac{\zeta - 1}{\zeta}\right)\left(\mathcal{P}\int_{-\infty}^{\infty} \mathrm{d}t\rho_0(t;\zeta)p_{n_1}(t;\zeta)p_{m_1}(t;\zeta)g^{\eta}_{n_2m_2}(t_0 - t) - \frac{\mathrm{i}}{2}(-1)^{n_1+m_1}g^{\eta}_{n_2m_2}(t_0)\right). \tag{87}$$

Further, combining (72) with (A.1) and (45), we can obtain another allowable sets of the parameters. For instance, $A_\xi = 1, x_n(t) = 2\pi\mathrm{i}\rho_0(t;\zeta), A_\eta = \frac{k}{\mathrm{i}\pi}, y_n(t) \equiv 0, B_n = D_n = 1$.

(b) $C \neq 0$

The elements of the matrix $\mathbf{G}(t_0; C)$ may be written as the convolution integral

$$G_{n_1n_2,m_1m_2}(t_0; C) = \int_{-\infty}^{\infty} \mathrm{d}s\, \tilde{g}^{\xi}_{n_1m_1}(t; C) g^{\eta}_{n_2m_2}(t_0 - t; C), \tag{88}$$

where $s = \frac{k}{\gamma}\left(t + \frac{\mathrm{i}}{2}\right)$ and $\tau = s - \frac{\mathrm{i}}{2}$ (see (49)). Here, the non-uniqueness of only $\mathbf{g}_{\xi}$ is taken into consideration for simplicity, i.e. $\tilde{g}^{\xi}_{nm}$ and g^{η}_{nm} are taken to be

$$\tilde{g}^{\xi}_{nm}(t; C) = \frac{\mathrm{i}}{2k}\left(\frac{\chi - 1}{\chi}\right)\frac{\theta^{n+m+1}}{\chi^m} p_{\nu}(\tau; \zeta)[A_{\xi} q_{\mu}(\tau; \zeta) + x_{\mu}(\tau) p_{\mu}(\tau; \zeta)]B_m, \tag{89}$$

$$g^{\eta}_{nm}(t_0 - t; C) = \frac{\mathrm{i}}{2k}\frac{(\chi - 1)\chi^m}{\theta^{n+m+1}} p_{\nu}\left(\tau - \frac{k}{\gamma}t_0; \zeta^{-1}\right) q_{\mu}\left(\tau - \frac{k}{\gamma}t_0; \zeta^{-1}\right). \tag{90}$$

The integration over s in (88) is performed on the assumption that s and C (γ) are independent of one another.

Allowable parameters A_{ξ}, $x_n(\tau)$ and B_m can be determined by substituting (88)–(90) into (80). For instance, putting $A_{\xi} = 0$ and $x_n(\tau) = 2k\rho(\tau; \zeta)$, we obtain $B_m = \frac{1}{\theta^{2m+1}}\frac{(\zeta-1)}{(\chi-1)}\left(\frac{\chi}{\zeta}\right)^{m+1}$. Thus the matrix elements of the two-dimensional Green's function can be written in the form

$$G_{n_1n_2,m_1m_2}(t_0; C) = \frac{\mathrm{i}}{\zeta^{m_1}}\left(\frac{\zeta - 1}{\zeta}\right)\theta^{n_1-m_1}\int_{-\infty}^{\infty} \mathrm{d}s\, \sigma(s; \zeta) p_{n_1}(\tau; \zeta) p_{m_1}(\tau; \zeta) g^{\eta}_{n_2m_2}(t_0 - t; C). \tag{91}$$

6. Conclusion

The six-dimensional Green's function matrix $\underline{\mathfrak{G}}$ can be expressed as a convolution integral

$$\underline{\mathfrak{G}} = \iint \mathrm{d}C_1 \mathrm{d}C_2 \mathbf{G}_1(t_{23}; \mu_{23}C_1) \otimes \mathbf{G}_2(t_{13}; \mu_{13}C_2) \otimes \mathbf{G}_3(t_{12}; -\mu_{12}(C_1 + C_2)) \tag{92}$$

over the separation constants C_1 and C_2 (the constraint (16) is taken into account). Here $\mathbf{G}_j(t_{ls}; \mu_{ls}C_j)$ are the two-dimensional Green's function matrices obtained in the previous section. Note that $C_j = -\frac{1}{2\mu_{ls}}\left(\gamma_j^2 - k_{ls}^2\right)$ plays the role of the energy. Before we can use the integral (92), we need to study the properties of $\mathbf{G}_j(t_{ls}; \mu_{ls}C_j)$ considered a functions of C_j. In particular, for $\mathbf{G}_j(t_{ls}; \mu_{ls}C_j)$ an analogue of the orthogonality relation (A1) should be obtained.

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Appendix. One useful orthogonality relation

In this appendix we derive the orthogonality relation

$$\frac{2\mathrm{i}k}{\pi}\int_{-\infty}^{\infty} \mathrm{d}t\, g^{\xi}_{nm}(t) = \delta_{nm}. \tag{A.1}$$

Using the integral representation (equation (15.3.1) in [13]) of the hypergeometric function in (37), we can rewrite the integral on the left-hand side of (A.1) in the form

$$\frac{1}{\pi}\left(\frac{\zeta}{\zeta-1}\right)^{\mu}\frac{1}{\zeta^{m}}\int_{0}^{1}\mathrm{d}x\,\frac{x^{\mu}}{\left(1-x\frac{\zeta}{\zeta-1}\right)^{\mu+1}}\int_{-\infty}^{\infty}\mathrm{d}t\,p_{\nu}(t;\zeta)\,\mathrm{e}^{-\mathrm{i}t\ln(1-x)}. \qquad (A.2)$$

Note that the integral over t in (A.2) consists of integrals

$$\int_{-\infty}^{\infty}\mathrm{d}t\,(-\mathrm{i}t)^{\ell}\,\mathrm{e}^{-\mathrm{i}t\ln(1-x)} = 2\pi\left[(x-1)\frac{\mathrm{d}}{\mathrm{d}x}\right]^{\ell}\delta(x), \qquad \ell\leqslant\nu\leqslant\mu, \qquad (A.3)$$

i.e. is expressed in terms of derivatives of the delta function. Further, introducing the function

$$y_{j}(x) = \frac{x^{\mu}(x-1)^{j}}{\left(1-x\frac{\zeta}{\zeta-1}\right)^{\mu+1}}, \qquad (A.4)$$

we obtain

$$\mathcal{I}_{j\ell} \equiv \int_{0}^{1}\mathrm{d}x\,y_{j}(x)\delta^{(\ell)}(x) = \begin{cases}\frac{1}{2}(-1)^{\ell}y_{j}^{(\ell)}(0) = \frac{\mu!}{2}(-1)^{\ell+j}, & \ell=\mu,\\ 0, & \ell<\mu.\end{cases} \qquad (A.5)$$

From (A.5) it follows that the integral in (A.2) is nonzero if $n = m(=\nu = \mu)$. In this case the only contribution to the integral comes from the leading term of the polynomial $p_n(t;\zeta)$ (which is equal to $\frac{1}{n!}(\zeta-1)^{n}(-\mathrm{i}t)^{n}$). Thus, we obtain for (A.2):

$$\frac{1}{\pi}\left(\frac{\zeta}{\zeta-1}\right)^{n}\frac{1}{\zeta^{n}}\frac{1}{n!}(\zeta-1)^{n}2\pi\mathcal{I}_{nn} = 1. \qquad (A.6)$$

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