Abstract

The possibility of using straight-line paths of integration in computing the integral representation of the three-body Coulomb Green’s function is discussed. In our numerical examples two different kinds of integration contours in the complex energy planes are considered. It is demonstrated that straight-line paths, which cross the positive real axis, are suitable for numerical computation.

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1. Introduction

In two previous papers [1, 2] a method was introduced as a new approach for solution of the three-body continuum problem using the infinite set of $L^2$ parabolic Sturmian basis functions for the wavefunction of the system. The goal of these papers has been the construction of exact analytic matrix elements of the three-body Coulomb Green’s function. The development of our method is based primarily upon the fact that for large particle separation the Schrödinger equation is separable in terms of generalized parabolic coordinates [3]. Thus, the corresponding six-dimensional resolvent operator can be expressed as a convolution of three two-dimensional Green’s functions $G_1$, $G_2$ and $G_3$. This representation involves integration along two contours $C^{(1)}$ and $C^{(2)}$, which encircle the spectra of two of the three two-dimensional wave operators (see, e.g., [4]).

Unfortunately, these (double) contour integrals are very inconvenient for numerical evaluation. Actually, to the contours $C^{(1)}$ and $C^{(2)}$ in the complex $\mathcal{E}_1$- and $\mathcal{E}_2$-planes there corresponds a domain in the $\mathcal{E}_3$-plane. Since the Green’s function $G_3$ is multivalued, this integration region in the complex $\mathcal{E}_3$-plane must possess a branch cut (along the positive real axis). Thus, to perform such integrals, one must provide an unambiguous prescription for selecting the appropriate branches of the Green’s function $G_3$. To do this one has to keep track of the trajectory defined by $\mathcal{E}_3$ ($\mathcal{E}_1$, $\mathcal{E}_2$) (as $\mathcal{E}_1$ and $\mathcal{E}_2$ move along the contours $C^{(1)}$ and
coordinates and present the associated Green’s function operator. However, such monitoring presents difficulties. It is preferable to employ straight-line paths of integration, such that \( C^{(1)} \) is parallel to \( C^{(2)} \), because in that case the domain of integration in the complex \( \mathcal{E}_3 \)-plane reduces to a straight line, and thus the appropriate single-valued integrand of the convolution integral can be easily produced. In this paper we wish to learn how to choose appropriate straight-line paths of integration which are suitable for numerical computation.

We outline below how the Schrödinger equation for a three-body Coulomb system is transformed into a Lippmann–Schwinger equation in terms of generalized parabolic coordinates and present the associated Green’s function operator.

The Schrödinger equation for three particles with masses \( m_1, m_1, m_3 \) and charges \( Z_1, Z_2, Z_3 \) is

\[
\left[ -\frac{1}{2\mu_1} \Delta_R - \frac{1}{2\mu_3} \Delta_r + \frac{Z_1Z_2}{r_{12}} + \frac{Z_2Z_3}{r_{23}} + \frac{Z_1Z_3}{r_{13}} \right] \Psi = E \Psi, \tag{1}
\]

where \( \mathbf{R} \) and \( \mathbf{r} \) are the Jacobi vectors

\[
\mathbf{R} = \mathbf{r}_1 - \mathbf{r}_2, \quad \mathbf{r} = \mathbf{r}_3 - \frac{m_1 \mathbf{r}_1 + m_2 \mathbf{r}_2}{m_1 + m_2}, \tag{2}
\]

\( r_{ls} = |\mathbf{r}_{ls}|, \mu_{12} \) and \( \mu_3 \) are the reduced masses

\[
\mu_{12} = \frac{m_1m_2}{m_1 + m_2}, \quad \mu_3 = \frac{m_3(m_1 + m_2)}{m_1 + m_2 + m_3}. \tag{3}
\]

The ansatz

\[
\Psi = e^{i\langle \mathbf{K} \cdot \mathbf{R} - \mathbf{k} \cdot \mathbf{r} \rangle / \Psi} \tag{4}
\]

removes the eigenenergy \( E = \frac{1}{2\mu_1} \mathbf{K}^2 + \frac{1}{2\mu_3} \mathbf{k}^2 \) giving the equation for \( \Psi \):

\[
\left[ -\frac{1}{2\mu_1} \Delta_R - \frac{1}{2\mu_3} \Delta_r - \frac{i}{\mu_{12}} \mathbf{K} \cdot \nabla_R - \frac{i}{\mu_3} \mathbf{k} \cdot \nabla_r + \frac{Z_1Z_2}{r_{12}} + \frac{Z_2Z_3}{r_{23}} + \frac{Z_1Z_3}{r_{13}} \right] \Psi = 0. \tag{5}
\]

Then, the operator in the square braces is expressed in terms of the generalized parabolic coordinates [3]:

\[
\xi_1 = r_{23} + \hat{\mathbf{k}}_{23} \cdot \mathbf{r}_{23}, \quad \eta_1 = r_{23} - \hat{\mathbf{k}}_{23} \cdot \mathbf{r}_{23},
\]

\[
\xi_2 = r_{13} + \hat{\mathbf{k}}_{13} \cdot \mathbf{r}_{13}, \quad \eta_2 = r_{13} - \hat{\mathbf{k}}_{13} \cdot \mathbf{r}_{13},
\]

\[
\xi_3 = r_{12} + \hat{\mathbf{k}}_{12} \cdot \mathbf{r}_{12}, \quad \eta_3 = r_{12} - \hat{\mathbf{k}}_{12} \cdot \mathbf{r}_{12}, \tag{6}
\]

where \( \mathbf{k}_{ls} = \frac{m_l - m_s}{m_l + m_s} \mathbf{k}_l \) is the relative momentum, \( \hat{\mathbf{k}}_{ls} = \mathbf{k}_{ls} / k_{ls} \) and \( k_{ls} = |\mathbf{k}_{ls}| \). In the resulting equation

\[
[\hat{D}_0 + \hat{D}_1] \Psi = 0, \tag{7}
\]

the first operator is given by

\[
\hat{D}_0 = \sum_{j=1}^{3} \frac{1}{\mu_{ls} (\xi_j + \eta_j)} [\hat{h}_{\xi_j} + \hat{h}_{\eta_j} + 2k_{ls} t_{ls}] \tag{8}
\]

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 \( \hat{h}_{\xi_j} \) and \( \hat{h}_{\eta_j} \) are

\[
\hat{h}_{\xi_j} = -2 \left( \frac{\partial}{\partial \xi_j} \xi_j \frac{\partial}{\partial \xi_j} + i k_{ls} \xi_j \frac{\partial}{\partial \xi_j} \right), \quad \hat{h}_{\eta_j} = -2 \left( \frac{\partial}{\partial \eta_j} \eta_j \frac{\partial}{\partial \eta_j} - i k_{ls} \eta_j \frac{\partial}{\partial \eta_j} \right). \tag{9}
\]

\( \hat{D}_0 \) is the leading term which provides a three-body continuum wavefunction that satisfies exact asymptotic boundary conditions for Coulomb systems, when the three particles are far
away from each other [3]. In turn, the operator $\hat{D}_1$ (which contains the non-orthogonal part of the kinetic energy operator) is regarded as a small perturbation which does not violate the boundary conditions.

The best known approximate solution to equation (7), the so-called C3 model [3, 5–7], is obtained by neglecting $\hat{D}_1$. Many improvements to the C3 model have been developed by considering in some approximate way of the neglected terms of the kinetic energy (see, e.g., [8] and references therein). In our approach the wavefunction $\Psi$ is obtained by solving an equivalent Lippman–Schwinger integral equation

$$\Psi = \Psi^{(0)} - \hat{G} \hat{V} \Psi.$$  \hspace{1cm} (10)

Here $\hat{G}$ plays the role of the Green’s function operator which is formally inverse to the six-dimensional operator $\hat{h}$ given by

$$\hat{h} = \prod_{j=1}^{3} \mu_{ls} (\xi_j + \eta_j) \hat{D}_0 = \mu_{13} (\xi_2 + \eta_2) \mu_{12} (\xi_3 + \eta_3) \hat{h}_1$$

\hspace{1cm} + $\mu_{23} (\xi_1 + \eta_1) \mu_{12} (\xi_3 + \eta_3) \hat{h}_2 + \mu_{23} (\xi_1 + \eta_1) \mu_{13} (\xi_2 + \eta_2) \hat{h}_3,$  \hspace{1cm} (11)

\hspace{1cm} $\hat{h}_j = \hat{h}_{\xi j} + \hat{h}_{\eta j} + 2k_{ls} t_{ls}$.  \hspace{1cm} (12)

In turn, the ‘potential’ $\hat{V}$ is defined as

$$\hat{V} = \prod_{j=1}^{3} \mu_{ls} (\xi_j + \eta_j) \hat{D}_1.$$  \hspace{1cm} (13)

The inhomogeneous term $\Psi^{(0)}$ of equation (10) can be taken as the wavefunction of the C3 model, i.e. expressed in terms of a product of three Coulomb waves.

It has been suggested in [1, 2] to treat the equation within the context of the $L^2$ parabolic Sturmian basis set [9]

$$|\Psi\rangle = \prod_{j=1}^{3} \phi_{n_j, m_j} (\xi_j, \eta_j).$$  \hspace{1cm} (14)

$$\phi_{n_j, m_j} (\xi_j, \eta_j) = \psi_{n_j} (\xi_j) \psi_{m_j} (\eta_j),$$  \hspace{1cm} (15)

$$\psi_n (x) = \sqrt{2b} e^{-bx} L_n (2bx),$$  \hspace{1cm} (16)

where $b$ is the scaling parameter. A solution $\Psi$ of the Lippman–Schwinger equation (10) is expanded in the basis (14) as

$$\Psi = \sum_{\eta_1} a_{\eta_1} |\eta_1\rangle.$$  \hspace{1cm} (17)

The discrete analog of the Lippman–Schwinger equation is obtained by putting (10) in the basis set (14). This yields

$$a = a^{(0)} - \mathcal{G} V a,$$  \hspace{1cm} (18)

where $\mathcal{G}$ and $V$ are the matrices of the operators $\hat{G}$ and $\hat{V}$ in the basis (14) and $a$ and $a^{(0)}$ are the coefficient vectors of $\Psi$ and $\Psi^{(0)}$, respectively.

It has been shown in our previous paper [2] that the matrix $\mathcal{G}$ can be represented in the form of a convolution integral

$$\mathcal{G}(\pm) = \frac{N}{(2\pi i)^2} \int_{C_1} \int_{C_2} \frac{d\xi_1}{\mu_{13}} \frac{d\xi_2}{\mu_{23}} G^{(\pm)} (t_{12}; \xi_1) \otimes G^{(\pm)} (t_{13}; \xi_2)$$

\hspace{1cm} $\otimes G^{(\pm)} (t_{12}; \xi_3 = \frac{k_{12}^2}{2} + \frac{\mu_{12}}{\mu_{23}} \left( \frac{k_{23}^2}{2} - \xi_1 \right) + \frac{\mu_{12}}{\mu_{13}} \left( \frac{k_{13}^2}{2} - \xi_2 \right)),$  \hspace{1cm} (19)

where $C_1$ and $C_2$ are the contours taken in the complex plane of the variables $\xi_1$ and $\xi_2$, respectively.
Here \( \mathbf{G}(t, \varepsilon) \) is the matrix which is inverse of the two-dimensional operator \( \hat{h}_j + \left( \frac{k_j^2}{2} - \varepsilon_j \right) (\xi_j + \eta_j) \) matrix representation in the basis (15), i.e.

\[
\left[ h_j + \left( \frac{k_j^2}{2} - \varepsilon_j \right) \right] \mathbf{G}(t, \varepsilon) = \mathbf{I}_j.
\]

Here the matrix \( h_j \) of the operator \( \hat{h}_j \) (12) is expressed in terms of the one-dimensional operators (9) matrices:

\[
h_j = h_{\xi j} \otimes I_{\eta j} + I_{\xi j} \otimes h_{\eta j} + 2k_j t_j I_j.
\]

In equations (20) and (21) \( I_{\xi j} \) and \( I_{\eta j} \) are unit matrices. \( Q_j = Q_{\xi j} \otimes I_{\eta j} + I_{\xi j} \otimes Q_{\eta j} \), where \( Q_{\xi j} \) and \( Q_{\eta j} \) are the matrices of \( \xi_j \) and \( \eta_j \) in the basis (16), respectively.

In this paper we make use of matrices \( \mathbf{G}(t, \varepsilon) \) (A.21) which are more symmetric (in \( \xi \) and \( \eta \)) than those obtained in our previous work [2]. The advantage of this representation of the two-dimensional Green’s function operator is that the convolution integral (A.21) can be performed in terms of hypergeometric functions (see for details appendix B). For simplicity of the notation, we omit indices for a while. The new matrix \( \mathbf{G}(t, \varepsilon) \) also obeys the completeness relation

\[
\frac{1}{2\pi i} \int_C \mathrm{d}\varepsilon \mathbf{G}(t, \varepsilon) = [Q_{\xi} \otimes I_{\eta} + I_{\xi} \otimes Q_{\eta}]^{-1}
\]

established in [2]. Here \( C \) is a contour originating at \( \varepsilon = \infty \), below the positive real axis rounding the lowest bound state \( \varepsilon_1 = -\frac{(kt)^2}{2\ell^2} \) for \( t < 0 \) (or the origin for \( t > 0 \)), and then heading back to \( \varepsilon = \infty \)—this time staying above the cut (see figure 1).

The integration contours of the convolution integral (19) \( \mathbf{C}^{(1,2)} \) are similar to the contour \( C \) (see, e.g., [4]). However, despite the known paths of integration representation (19) poses difficulties in a practical application. Actually, from the relationship

\[
\varepsilon_3 = \frac{k_{12}^2}{2} + \frac{\mu_{12}}{\mu_{23}} \left( \frac{k_{23}^2}{2} - \varepsilon_1 \right) + \frac{\mu_{12}}{\mu_{13}} \left( \frac{k_{13}^2}{2} - \varepsilon_2 \right) + \mu_{12} \left( \frac{k_{1}^2}{2} - \varepsilon_0 \right) + \mu_{12} \left( \frac{k_{2}^2}{2} - \varepsilon_0 \right) + \mu_{12} \left( \frac{k_{3}^2}{2} - \varepsilon_0 \right)
\]

it is easy to see that the domain of integration in the complex \( \varepsilon_3 \)-plane is represented as a semi-infinite rectangle (the hatched zone in figure 2) with the cut from its right edge \( (x_0 = \frac{k_{1}^2}{2} + \varepsilon_0 + \varepsilon_{10} + \varepsilon_{20}) \) to the origin. Thus, as \( \varepsilon_1 \) and \( \varepsilon_2 \) proceed along their contours \( C^{(1)} \) and \( C^{(2)} \), the corresponding point in the \( \varepsilon_3 \)-plane crosses the cut
and moves from one sheet (e.g. the ‘physical’ energy sheet \(0 \leq \text{arg}(\mathcal{E}_3) < 2\pi\)) to another (the ‘unphysical’ energy sheet \(-2\pi \leq \text{arg}(\mathcal{E}_3) < 0\)). If the integrand involves a multivalued function, care must be taken with the cut in the integration region. In our case, the problem is how to trace crossing the cut in the \(\mathcal{E}_3\)-plane (and determine \(\text{arg}(\mathcal{E}_3)\)) during numerical integration over \(\mathcal{E}_1\) and \(\mathcal{E}_2\).

The numerical evaluation of integral (19) can be simplified considerably by using parallel lines as paths of integration \(C^{(1)}\) and \(C^{(2)}\), since, in this case the argument of the energy \(\mathcal{E}_3\) is uniquely determined by its imaginary part sign. In this paper we wish to learn how to choose appropriate straight-line paths \(C^{(1)}\) and \(C^{(2)}\) for which the integral representation (19) is valid. Unfortunately, the contour integrals of interest cannot be treated analytically, so we must resort to numerical experiments.

The numerical examples presented in section 3 show that the contour \(C\) in (22) could be deformed so that it becomes the disconnected pair of straight lines. The value of the integral over each of these straight-line paths is half the value of the contour integral (22). In this section we consider two kinds of straight-line paths. In section 4 based upon the numerical results obtained for double integrals which arise from the matrix product \(\hbar \mathcal{G}(\mathcal{E}_j)\), we find the straight-line contours \(C^{(1,2)}\) providing a non-zero integral representation (19). Section 5 contains a brief discussion of the overall results. For completeness we review briefly the results of our previous works [1, 2] in appendix A. Details concerning the evaluation of matrix elements of the two-dimensional Green’s function operator are given in appendix B.

2. Preliminaries

We assume that the relationships between contour integrals obtained in this work depend only upon the intrinsic properties of the Green’s function itself (and are independent of the base function (14) numbers that specify indices of the matrix elements of the operators). Thus, in all our numerical examples (except for the case where the inverse relationship between \(\hbar\) and \(\mathcal{G}\) is demonstrated) we only use the element \(G_{0,0,0}^{(+)}(t_\nu; \mathcal{E}_j)\) (see equation (B.10) in appendix B) of the matrices \(G^{(+)}(t_\nu; \mathcal{E}_j)\). For \(n = m = 0\) we have from equation (B.10) that

\[
G_{0}^{(+)}(t; \mathcal{E}) \equiv G_{0,0,0}^{(+)}(t; \mathcal{E}) = \frac{i}{2\gamma} \left(\frac{\zeta - 1}{\zeta}\right) \frac{1}{1 + i\tau} 2F_1(1, i\tau; 2 + i\tau; \zeta^{-1}).
\]
where\[
E = \frac{\gamma^2}{2}, \quad \tau = \frac{k}{\gamma},
\]
and\[
\zeta = \frac{\lambda}{\theta}, \quad \theta = \frac{2b + i(y - k)}{2b - i(y - k)}, \quad \lambda = \frac{2b - i(y + k)}{2b + i(y + k)}.\]

(26)

For \(\text{Im}(\gamma) > 0\) we have \(|\zeta| > 1\), and therefore the Gauss hypergeometric function in (24) is absolutely convergent (see, e.g., [11]). Thus, equation (24) serves as a definition of the Green’s function in the upper half of the complex \(\gamma\)-plane. If \(\gamma\) happens to have a negative imaginary part, then \(|\zeta| < 1\) and the linear transformation formula (15.3.7) in [11] can be used to define the Green’s function \(G_0^{(+)}\) in the lower half-plane. Actually, this transformation of the hypergeometric function on the right-hand side of (24) let us write

\[
G_0^{(+)}(t; E) = \frac{i}{2\gamma} (\zeta - 1) \left\{ \frac{1}{1 - i\tau} \, _2F_1(1, -i\tau; 2 - i\tau; \zeta) - \left(\frac{\zeta - 1}{\zeta}\right)^{i\tau} \Gamma(1 + i\tau) \Gamma(1 - i\tau) \right\}.\]

(27)

Here, the hypergeometric series is again absolutely convergent.

The function \(E = \frac{\gamma^2}{2}\) maps the upper half of the complex \(\gamma\)-plane into the entire complex \(E\)-plane with the cut along the positive real axis. In turn, simple poles of the Green’s function on the positive part of the imaginary axis at \(\gamma_\ell = -i\ell\frac{b}{\gamma}, \ell = 1, 2, \ldots\), for \(t < 0\) are mapped onto points \(E^{(+)} = -\frac{4\ell^2}{\gamma^2}\) on the negative real axis in the complex energy plane.

Note that using the integral representation (15.3.1) in [11] of the hypergeometric function one can increase greatly the radius of convergence of the Gauss series (in fact, (15.3.1) serves as a definition of \(_2F_1(a, b; c; z)\) for \(\text{Re}(c) > \text{Re}(b) > 0\) in the complex \(z\)-plane with the cut along the real axis from 1 to \(\infty\)). The same is also true for the Gauss continued fraction representation [10] of the hypergeometric functions which has been used in our calculations. The results presented in tables 1 and 2 show that this approximation provides a reasonable accuracy.

The completeness relation (22) for \(G_0^{(+)}(t; E)\) takes the form

\[
\frac{1}{2\pi i} \oint_{cE} dE \, G_0^{(+)}(t; E) = 2b.
\]

(28)

This result is numerically obtained by evaluating the contour integral on the left-hand side of (28). Note that the value of the integral represents the matrix element \([Q^{-1}]_{0,0,0,0}\) of \(Q^{-1}\), which is the inverse of the infinite matrix \(Q \equiv Q_\xi \otimes I_\eta + I_\xi \otimes Q_\eta\). All the integrals in this paper are computed using IMSL FORTRAN Library routines.

In this paper numerical experiments are performed with different sets of physical parameters \(\{Z_j, m_j, k_{\ell j}, j = 1, 3\}\) and for different values of the scaling parameter \(b\). For simplicity the atomic units \(\hbar = c = 1\) are employed.

3. Straight-line paths

Let us deform the contour \(C\) by moving its left edge toward minus infinity so that it becomes the disconnected pair of straight lines (\(C_1\) and \(C_2\) in figure 1) parallel to the real axis. It should be noted that one must be careful while deforming contours of infinite length because the Cauchy–Goursat theorem on the path-independence of integrals of analytic functions was
Table 1. The numerical results obtained for integrals $v_0^{(1)}$ (38) and $v_0^{(3)}$ (40) along the contours $C_1$ and $C_3$, respectively.

| $b$ | $t$ | $v_0^{(1)}$ | $v_0^{(3)}$ |
|-----|-----|-------------|-------------|
|     |     | Contour $C_1$: $\mathcal{E} = y_0 + x$ | Contour $C_3$: $\mathcal{E} = \frac{k}{\mu} + iy$ |
|     |     | $k = 1.5$ | $k = 0.1$ |
|     |     | $y_0 = 50$ | $y_0 = 100$ |
| 1   | $\frac{2}{7}$ | $0.99999999 - i 0.591157585 \times 10^{-8}$ | $0.99999999 + i 0.81801613 \times 10^{-8}$ |
|     |     | $y_0 = 100$ | $y_0 = 100$ |
|     |     | $0.99999999 - i 0.59144067 \times 10^{-8}$ | $0.99999999 - i 0.89459450 \times 10^{-8}$ |
|     |     | $y_0 = 500$ | $y_0 = 500$ |
|     |     | $0.99999999 - i 0.59117013 \times 10^{-8}$ | $0.99999999 - i 0.95821632 \times 10^{-8}$ |
|     |     | $k = 1$ | $k = 10$ |
| 2   | $\frac{2}{7}$ | $1.99999998 - i 0.22924528 \times 10^{-7}$ | $1.99999999 + i 0.14828515 \times 10^{-7}$ |
|     |     | $1.99999998 - i 0.22921813 \times 10^{-7}$ | $1.99999999 - i 0.19451100 \times 10^{-7}$ |
|     |     | $1.99999998 - i 0.23123753 \times 10^{-7}$ | $1.99999999 + i 0.11624553 \times 10^{-7}$ |
|     |     | $1.99999998 - i 0.22916396 \times 10^{-7}$ | $1.99999999 - i 0.16220747 \times 10^{-7}$ |
| 5   | $\frac{2}{7}$ | $4.99999986 - i 0.457255740 \times 10^{-7}$ | $4.99999997 + i 0.25717124 \times 10^{-7}$ |
|     |     | $4.99999986 - i 0.45733516 \times 10^{-7}$ | $4.99999997 - i 0.60004389 \times 10^{-7}$ |
|     |     | $4.99999986 - i 0.45738397 \times 10^{-7}$ | $4.99999997 + i 0.17642813 \times 10^{-7}$ |
|     |     | $4.99999986 - i 0.45748507 \times 10^{-7}$ | $4.99999997 - i 0.51933984 \times 10^{-7}$ |
The numerical results obtained for double integrals (59), (62) and (60) along the contours $C_1$ and $C_3$ and for the element $[h(\mathcal{E}^{(s)})]_{0,0}$ of the matrix product $h(\mathcal{E}^{(s)})$.

| Contour $C_1$ | Contour $C_3$ |
|----------------|----------------|
| $E_1 = 1y_0 + x_1$, $E_2 = 1y_0 + x_2$, $y_0 = 100$ | $E_1 = \frac{e_i^2}{2} + iy_1$, $E_2 = \frac{e_i^2}{2} + iy_2$ |
| $Z_1 = Z_2 = -1$, $Z_3 = 2$, $m_1 = m_2 = 1$, $m_3 = \infty$, $k_{23} = k_{13} = k_{12} = 1.5$, $b = 1$ | |
| $w_1 = -0.500000080 - i0.2130977 \times 10^{-5}$ | $w_1 = 1.50000035 - i0.99107240 \times 10^{-5}$ |
| $w_2 = -0.50000885 + i0.393861 \times 10^{-6}$ | $w_2 = 1.49999966 - i0.10095533 \times 10^{-4}$ |
| $w_3 = 0.99999999 - i0.48919801 \times 10^{-8}$ | $w_3 = 1.00000000 - i0.32751568 \times 10^{-9}$ |
| $I_0 = 0.14447467 \times 10^{-11} + i0.10094339 \times 10^{-11}$ | $h(\mathcal{E}^{(s)})_{0,0} = 1.00000000 - i0.83521957 \times 10^{-10}$ |
| $Z_1 = 2$, $Z_2 = -2$, $Z_3 = 10$, $m_1 = 1$, $m_2 = 2$, $m_3 = 3$, $k_{23} = 5$, $k_{13} = 10$, $k_{12} = 2$, $b = 5$ | |
| $w_1 = -0.26625080 + i0.51119007 \times 10^{-5}$ | $w_1 = 1.73374726 - i0.12106662 \times 10^{-4}$ |
| $w_2 = 0.73375735 - i0.62155073 \times 10^{-5}$ | $w_2 = 1.26625077 + i0.82543780 \times 10^{-4}$ |
| $w_3 = 0.99999655 - i0.34672801 \times 10^{-5}$ | $w_3 = 0.99999999 - i0.49043120 \times 10^{-5}$ |
| $I_0 = 0.44233553 \times 10^{-5} + i0.10375885 \times 10^{-8}$ | $h(\mathcal{E}^{(s)})_{0,0} = 1.00000000 + i0.15785475 \times 10^{-6}$ |
| $Z_1 = -1$, $Z_2 = 2$, $Z_3 = 10$, $m_1 = 1$, $m_2 = 5$, $m_3 = 10$, $k_{23} = 3$, $k_{13} = 5$, $k_{12} = 7$, $b = 3$ | |
| $w_1 = -0.11147116 + i0.71622550 \times 10^{-6}$ | $w_1 = 1.88852574 - i0.32953979 \times 10^{-5}$ |
| $w_2 = -0.88852896 + i0.26680011 \times 10^{-5}$ | $w_2 = 1.11147154 - i0.20944638 \times 10^{-5}$ |
| $w_3 = 0.99999790 - i0.20913236 \times 10^{-6}$ | $w_3 = 0.99999999 - i0.81986763 \times 10^{-6}$ |
| $I_0 = 0.39551033 \times 10^{-10} - i0.34011037 \times 10^{-10}$ | $h(\mathcal{E}^{(s)})_{0,0} = 0.99999986 + i0.21420294 \times 10^{-6}$ |
derived for finite contours. In this case, we claim that the deformation above does not alter the value of the integral

$$v_{n;m'} = \frac{1}{2\pi i} \int_{C} d\xi G^{(s)}_{nm'; n'm'} (t; \xi)$$  \hspace{1cm} (29)

and hence, $v_{n;m'}$ is divided into two contributions:

$$v_{n;m'} = v^{(1)}_{n;m'} + v^{(2)}_{n;m'},$$  \hspace{1cm} (30)

where

$$v^{(1)}_{n;m'} = \frac{1}{2\pi i} \int_{C_1} d\xi G^{(s)}_{nm'; n'm'} (t; \xi),$$  \hspace{1cm} (31)

$$v^{(2)}_{n;m'} = \frac{1}{2\pi i} \int_{C_2} d\xi G^{(s)}_{nm'; n'm'} (t; \xi).$$  \hspace{1cm} (32)

In order to check the claim, consider the contour integrals $v^{(1)}_{0}$ (31) and $v^{(2)}_{0}$ (32). Here, the energy $E$ is parametrized by $E = \gamma_{0} + x$ ($E = -i\gamma_{0} + x$), where the parameter $\gamma_{0}$ specifies the position of $C_{1}$ ($C_{2}$) with respect to the real axis (see figure 1). For large values of $|\gamma|$ the Green’s function (24) behaves as

$$G^{(s)}_{0} (t; \xi) \approx \frac{i}{2\gamma} \left( \frac{\xi - 1}{\xi} \right) = \frac{2b}{\gamma^2 + 4ib\gamma - (4b^2 + k^2)} \approx \frac{2b}{E},$$  \hspace{1cm} (33)

i.e. function (24) possesses the general property of the Green’s functions for large energies. Thus, in view of (33), for large $\gamma_{0}$ the real $A(x)$ and imaginary $B(x)$ parts of $\frac{1}{2\pi i} G^{(s)}_{0} (t; \xi)$, e.g., in the case of $C_{1}$, are

$$A(x) \approx \frac{b}{\pi} \frac{y_0}{y_0^2 + x^2}, \hspace{1cm} B(x) \approx \frac{b}{\pi} \frac{x}{y_0^2 + x^2},$$  \hspace{1cm} (34)

and therefore

$$v^{(1)}_{0} \approx \int_{-\infty}^{\infty} dx \frac{b}{\pi} \frac{y_0}{y_0^2 + x^2} + i \int_{-\infty}^{\infty} dx \frac{b}{\pi} \frac{x}{y_0^2 + x^2} = b.$$  \hspace{1cm} (35)

In a similar way, we obtain

$$v^{(2)}_{0} \approx b \hspace{1cm} \text{for large} \hspace{0.2cm} \gamma_{0}.$$  \hspace{1cm} (36)

Thus, at least for sufficiently large $\gamma_{0}$, the contour $C$ can be deformed, such that $C \rightarrow C_{1} + C_{2}$, without changing the value of the contour integral (28), and the integrals $v^{(1)}_{0}$ and $v^{(2)}_{0}$ are equal:

$$v^{(1)}_{0} = v^{(2)}_{0} = \frac{1}{2} v_{0}. $$  \hspace{1cm} (37)

Note that the Green’s function (24) decreases to zero as $|\xi| \rightarrow \infty$ too slowly (see (33)) for the integrals $v^{(1)}_{0}$ and $v^{(2)}_{0}$ to converge absolutely. The same is true for the double integrals (considered in the next section) whose integrands contain a product of two two-dimensional Green’s functions. Fortunately, the convolution integrals (19) converge absolutely, since the integrands of $G^{(ab)}$ decay fast enough at infinity.

The numerical results for the integrals

$$v^{(1)}_{0} = \int_{-\infty}^{\infty} dx \frac{1}{2\pi i} G^{(s)}_{0} (t; iy_{0} + x)$$  \hspace{1cm} (38)

with different $y_0$ are presented in table 1. Note that in the case of $C_{1}$ the integrand $\frac{1}{2\pi i} G^{(s)}_{0} (t; \xi)$ is a rather smooth function of the integration variable, as seen in figure 3. Thus, we have
a numerical confirmation of the validity of formula (37). Furthermore, it can be checked numerically that

\[ v^{(1)}_{nm; n'm'} = v^{(2)}_{nm; n'm'} = \frac{1}{2} v_{nm; n'm'} \]  

holds for arbitrary \( n, m, n', m' \).

Another straight-line path is obtained by rotating the contour \( \mathcal{C}_1 \) about some point \( x_0 \) on the positive real axis through an angle \( \varphi \) in the range \( -\pi < \varphi < 0 \) [2, 12]. For definiteness, we choose \( x_0 = \frac{E_0}{2 \tau} \) and \( \varphi = -\frac{\pi}{2} \), i.e. \( E = \frac{E_0}{2} + i y \) on the resulting contour \( \mathcal{C}_3 \), shown in figure 4. The path \( \mathcal{C}_3 \) crosses the cut so that its lower part (depicted in figure 4 by a dashed line) descends into the unphysical sheet \( -2\pi \leq \arg(E) < 0 \). To analytically continue \( G_0^{(s)} \) onto the unphysical sheet we use formula (27). Note that the numerical result for the integral

\[ v^{(3)}_0 = \frac{1}{2\pi} \int_{-\infty}^{\infty} dy G_0^{(s)} (t; \frac{k^2}{2} + i y) \]  

presented in table 1 also satisfies

\[ v^{(3)}_0 = \frac{1}{2} v_0. \]

Thus, we find another straight-line path \( \mathcal{C}_3 \) for which

\[ v^{(3)}_{nm; n'm'} = \frac{1}{2\pi} \int_{\mathcal{C}_3} dE G_0^{(s)} (t; E) = \frac{1}{2} v_{nm; n'm'}. \]

In table 1 the numerical results, obtained for integrals (38) and (40) with different values of \( k, t \) and \( b \), are presented. Note that these results confirm the validity of the formula

\[ v^{(1)}_0 = v^{(3)}_0 = b. \]
4. Double integrals

Now that we have relationships (39) and (42) between the integrals along the contour $C$ and the integrals over the straight-line paths, we can use paths of the types $C_1$ and $C_3$ in the integral representation (19) of the Green’s function operator. Before proceeding, we consider the matrix product $\mathbf{h} \mathcal{G}^{(+)}$ to determine the normalizing factors $\mathcal{N}$ corresponding to the $C_1$- and $C_3$-type paths. Using the six-dimensional operator $\hat{\mathbf{h}}$ (11) matrix representation

$$\hat{\mathbf{h}} = \mu_{12} \mu_{23} \mathbf{1}_1 \otimes \mathbf{Q}_2 \otimes \mathbf{Q}_3 + \mu_{23} \mu_{12} \mathbf{1}_2 \otimes \mathbf{Q}_1 \otimes \mathbf{Q}_3 + \mu_{12} \mu_{23} \mathbf{1}_3 \otimes \mathbf{Q}_2 \otimes \mathbf{h}_3,$$

(44)

and (19) and (20), we have

$$\mathbf{h} \mathcal{G}^{(+)} = \mathcal{N} \{ W_1 + W_2 + W_3 \},$$

(45)

where

$$W_1 = \frac{1}{(2\pi)^2} \int_{C_1} \int_{C_2} d\mathcal{E}_1 d\mathcal{E}_2 \mathbf{1}_1 \otimes [\mathbf{Q}_2 \mathcal{G}^{(+)}(t_{13}; \mathcal{E}_2)] \otimes \left[ \mathbf{Q}_3 \mathcal{G}^{(+)}(t_{23}; \mathcal{E}_3) \right],$$

(46)

$$W_2 = \frac{1}{(2\pi)^2} \int_{C_1} \int_{C_2} d\mathcal{E}_1 d\mathcal{E}_2 \mathbf{1}_2 \otimes [\mathbf{Q}_1 \mathcal{G}^{(+)}(t_{23}; \mathcal{E}_1)] \otimes \mathbf{1}_2,$$

(47)

$$W_3 = \frac{1}{(2\pi)^2} \int_{C_1} \int_{C_2} d\mathcal{E}_1 d\mathcal{E}_2 \left[ \mathbf{Q}_1 \mathcal{G}^{(+)}(t_{23}; \mathcal{E}_1) \right] \otimes \left[ \mathbf{Q}_2 \mathcal{G}^{(+)}(t_{13}; \mathcal{E}_2) \right] \otimes \mathbf{1}_3.$$  

(48)

The matrices $\mathbf{h}$ and $\mathcal{G}^{(+)}$ must be inverses of each other. Therefore, the normalizing factor $\mathcal{N}$ and the matrices $W_j$, $j = 1, 3$, satisfy the condition

$$\mathcal{N} \{ W_1 + W_2 + W_3 \} = \mathbf{I}.$$  

(49)

If we choose $C^{(1)}$ and $C^{(2)}$ paths to be of the same type ($C_1$ or $C_3$), then it follows from (22) and (39) (or (42)) that

$$W_3 = \frac{1}{4} \mathbf{1}_1 \otimes \mathbf{1}_2 \otimes \mathbf{1}_3 = \frac{1}{4} \mathbf{I}.$$  

(50)
Further, we assume that

\[ W_1 = \frac{\alpha}{4} \mathbf{I}, \quad W_2 = \frac{\beta}{4} \mathbf{I}, \]

so that the sum \( \{W_1 + W_2 + W_3\} \) is proportional to the unit matrix \( \mathbf{I} \). In turn, the constants \( \alpha \) and \( \beta \) can be determined by, e.g., the ratios

\[ \alpha = \frac{w_1}{w_3}, \quad \beta = \frac{w_2}{w_3}, \]

where

\[ w_1 = \frac{1}{(2\pi i)^2} \frac{\mu \lambda_2}{\mu_23} \int_{c_1} \int_{c_2} d\xi_1 d\xi_2 G_0^{(1)}(t_{13}; \xi_2) \]
\[ \times G_0^{(1)}(t_{12}; \xi_1; \frac{k_{12}^2}{2} + \frac{\mu_12}{\mu_23} (k_{23}^2/2 - \xi_1)), \]
\[ w_2 = \frac{1}{(2\pi i)^2} \frac{\mu \lambda_2}{\mu_23} \int_{c_1} \int_{c_2} d\xi_1 d\xi_2 G_0^{(1)}(t_{23}; \xi_1) \]
\[ \times G_0^{(1)}(t_{12}; \xi_1; \frac{k_{12}^2}{2} + \frac{\mu_12}{\mu_23} (k_{23}^2/2 - \xi_1)), \]
\[ w_3 = \frac{1}{(2\pi i)^2} \int_{c_1} \int_{c_2} d\xi_1 d\xi_2 G_0^{(1)}(t_{13}; \xi_1) G_0^{(1)}(t_{13}; \xi_2). \]

Thereafter, the normalizing factor \( N \) is expressed as

\[ N = \frac{4}{1 + \alpha + \beta}. \]

First we consider the path of the type \( C_1 \).

4.1. \( C^{(1)} \) and \( C^{(2)} \) are of the type \( C_1 \)

In this case the energies \( \xi_1 \) and \( \xi_2 \) are parametrized by \( \xi_1 = iy_{10} + x_1 \) and \( \xi_2 = iy_{20} + x_2 \) with \( y_{10}, y_{20} > 0 \). Hence, we have for the energy \( \xi_3 \)

\[ \xi_3 = -iy_{30} + x_3, \]

where

\[ y_{30} = \frac{\mu_12}{\mu_23} y_{10} + \frac{\mu_12}{\mu_{13}} y_{20}, \]
\[ x_3 = \frac{k_{12}^2}{2} + \frac{\mu_12}{\mu_23} (\frac{k_{23}^2}{2} - x_1) + \frac{\mu_12}{\mu_{13}} (\frac{k_{13}^2}{2} - x_2). \]

Assuming that the energy \( \xi_3 \) lies on the physical sheet i.e. \( 0 \leq \arg(\xi_3) < 2\pi \), in view of (37), (38), (55) and (56), we obtain that

\[ \frac{1}{2\pi i} \int_{-\infty}^{\infty} dx_1 G_0^{(1)}(t_{12}; -iy_{30} + x_3) = -\frac{\mu_23}{\mu_12} \frac{1}{2\pi i} \int_{-\infty}^{\infty} dx_3 G_0^{(1)}(t_{12}; -iy_{30} + x_3) \]
\[ = -\frac{\mu_23}{\mu_12} \frac{1}{2\pi i} \int_{C_1} d\xi G_0^{(1)}(t_{12}; \xi) = -\frac{\mu_23}{\mu_12} v_0^{(2)} = -\frac{\mu_23}{\mu_12} v_0^{(1)}. \]

Similarly,

\[ \frac{1}{2\pi i} \int_{-\infty}^{\infty} dx_2 G_0^{(1)}(t_{12}; -iy_{30} + x_3) = -\frac{\mu_13}{\mu_12} \frac{1}{2\pi i} \int_{C_1} d\xi G_0^{(1)}(t_{12}; \xi) = -\frac{\mu_13}{\mu_12} v_0^{(2)}. \]
Hence, one might expect that the constants $\alpha$ and $\beta$ (52) are negative. Note that in our case the integrals $w_j$ (53) take the forms

$$w_1 = \frac{1}{(2\pi i)^2} \frac{\mu_{12}}{\mu_{23}} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} dx_1 dx_2 \ G_0^{(s)}(t_{13}; i\omega_1 + \omega_2) \ G_0^{(t)}(t_{12}; -i\omega_3 + \omega_4),$$

$$w_2 = \frac{1}{(2\pi i)^2} \frac{\mu_{12}}{\mu_{13}} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} dx_1 dx_2 \ G_0^{(s)}(t_{23}; i\omega_1 + \omega_3) \ G_0^{(t)}(t_{12}; -i\omega_3 + \omega_4),$$

$$w_3 = \frac{1}{(2\pi i)^2} \frac{1}{\mu_{12} \mu_{13}} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} dx_1 dx_2 \ G_0^{(s)}(t_{23}; i\omega_1 + \omega_3) \ G_0^{(t)}(t_{13}; i\omega_2 + \omega_4).$$

In our calculations we put $\omega_1 = \omega_2 = \omega_3 = 100$. From the numerical results for the double integrals (59) presented in table 2, it follows that $\frac{\mu_1}{\mu_2} + \frac{\mu_2}{\mu_3} = -\frac{\mu_1}{\mu_3}$. Note that the same result is obtained using the approximation $G_0^{(s)}(t; \mathcal{E}) \approx \frac{2}{\mathcal{E}}$, valid for large $\mathcal{E}$ (see equation (33)). In this case the double integrals (59) are simple enough to evaluate symbolically. Thus, we have $\alpha + \beta + 1 = 0$, and so equation (54) is meaningless. This outcome is consistent with the numerical result obtained for the integral in expression (19) for the diagonal matrix element of $[\tilde{G}^{(s)}(t)]_{0,0}$ corresponding to the basis function $| \tilde{n} \rangle \equiv | n_j = m_j = 0, \ j = \mathbb{T}, \mathbb{I} \rangle$ (14):

$$I_0 = \frac{1}{(2\pi i)^2} \frac{1}{\mu_{12} \mu_{13}} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} dx_1 dx_2 \ G_0^{(s)}(t_{23}; i\omega_1 + \omega_3) \ G_0^{(t)}(t_{13}; i\omega_2 + \omega_4),$$

which is presented in table 2. Therefore, we conclude that paths of the type $C_1$ cannot be used in the integral representation (19).

Now consider contours of the type $C_3$.

4.2. $C^{(1)}$ and $C^{(2)}$ are of the type $C_3$

Here the energies $\mathcal{E}_1$ and $\mathcal{E}_2$ are given by $\mathcal{E}_1 = \frac{k_1^2}{2} + i\omega_1$ and $\mathcal{E}_2 = \frac{k_2^2}{2} + i\omega_2$. In turn, the energy $\mathcal{E}_3$ is parametrized as $\mathcal{E}_3 = \frac{k_3^2}{2} - i\omega_3$ with $\omega_3 = \frac{\mu_{13}}{\mu_{12}} \omega_1 + \frac{\mu_{13}}{\mu_{12}} \omega_2$. Note that from (40) it follows that

$$\frac{1}{2\pi} \int_{-\infty}^{\infty} dy_1 \ G_0^{(s)}(t_{12}; \frac{k_1^2}{2} - i\omega_3) = \frac{\mu_{13}}{\mu_{12}} \frac{1}{2\pi} \int_{-\infty}^{\infty} dy_3 \ G_0^{(s)}(t_{12}; \frac{k_3^2}{2} - i\omega_3),$$

$$\frac{1}{2\pi} \int_{-\infty}^{\infty} dy_2 \ G_0^{(s)}(t_{12}; \frac{k_2^2}{2} + i\omega_3) = \frac{\mu_{13}}{\mu_{12}} \frac{1}{2\pi} \int_{-\infty}^{\infty} dy_3 \ G_0^{(s)}(t_{13}; \mathcal{E} = \frac{\mu_{13}}{\mu_{12}} \omega_3),$$

$$\left( \frac{1}{2\pi} \int_{-\infty}^{\infty} dy_2 \ G_0^{(s)}(t_{12}; \frac{k_2^2}{2} - i\omega_3) = \frac{\mu_{13}}{\mu_{12}} \frac{1}{2\pi} \int_{-\infty}^{\infty} dy_3 \ G_0^{(s)}(t_{13}; \mathcal{E} = \frac{\mu_{13}}{\mu_{12}} \omega_3) \right).$$

Therefore, in contrast to the previous case, $w_1$ ($w_2$) would be expected to have the same sign as $w_3$. 

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In this case the contour integrals (53) are transformed into the double integrals
\[
\begin{align*}
w_1 &= \frac{1}{(2\pi)^2} \frac{\mu_{12}}{\mu_{23}} \int_{-\infty}^{+\infty} d\gamma_1 \int_{-\infty}^{+\infty} d\gamma_2 \ G_0^{(s)}(t_{13}; \frac{k_{12}^2}{2} + i\gamma_2) \ G_0^{(s)}(t_{12}; \frac{k_{12}^2}{2} - i\gamma_3), \\
w_2 &= \frac{1}{(2\pi)^2} \frac{\mu_{12}}{\mu_{23}} \int_{-\infty}^{+\infty} d\gamma_1 \int_{-\infty}^{+\infty} d\gamma_2 \ G_0^{(s)}(t_{23}; \frac{k_{23}^2}{2} + i\gamma_1) \ G_0^{(s)}(t_{12}; \frac{k_{12}^2}{2} - i\gamma_3), \\
w_3 &= \frac{1}{(2\pi)^2} \frac{\mu_{12}}{\mu_{23}} \int_{-\infty}^{+\infty} d\gamma_1 \int_{-\infty}^{+\infty} d\gamma_2 \ G_0^{(s)}(t_{23}; \frac{k_{23}^2}{2} + i\gamma_1) \ G_0^{(s)}(t_{13}; \frac{k_{13}^2}{2} + i\gamma_2),
\end{align*}
\]

From the numerical results for integrals (62), shown in table 2, it follows that \(\frac{w_1}{w_2} = \frac{w_2}{w_3} = \frac{3}{2\pi}\). Hence, \(\alpha + \beta + 1 = 4\) and \(\kappa = 1\). The same result can be obtained more easily using the limiting behavior (33) of \(G_0^{(s)}\) when the wavenumbers \(k_i\) assume extreme values.

To verify that the straight-line path of the type \(C_3\) does provide the desired result, we numerically evaluate the matrix elements
\[
[\theta^{(s)}]_{n_1, n_2} = \frac{1}{(2\pi)^2} \frac{1}{\mu_{23} \mu_{13}} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} d\gamma_1 \ d\gamma_2 \ G_{n_1, m_1; n_1', m_1'}^{(s)}(t_{13}; \frac{k_{13}^2}{2} + i\gamma_2) \ G_{n_2, m_2; n_2', m_2'}^{(s)}(t_{12}; \frac{k_{12}^2}{2} - i\gamma_3)
\]
and calculate the matrix product \(\hbar \theta^{(s)}\) of finite size. Note that the matrix \(\hbar (44)\) is ‘tridiagonal’, i.e. for each pair of indices \([n_j, n'_j]\) and \([m_j, m'_j]\), \(j = 1, 3\), the elements \([\theta]\) vanish unless \(|n_j - n'_j| \leq 1\) and \(|m_j - m'_j| \leq 1\). Therefore, the minimal rank \(N_{\min}\) of the matrices \(\hbar\) and \(\theta\), with which the relation \(\hbar \theta = 1\) could be verified, is given by \(N_{\min} = 2^8 = 64\). Actually, to test this equality, we must use all the basis functions \([\Phi]\) (14) with each of the \(n_j\) and \(m_j\) taking the value one or zero. Our prime interest here is with the values of the first row elements \([\hbar \theta^{(s)}]_{0, 0}\) in the matrix \(\hbar \theta^{(s)}\). The numerical results for the first diagonal element \([\hbar \theta^{(s)}]_{0, 0}\), obtained with different sets \([Z_j, m_j, k_{ij}, j = 1, 3, b]\), are presented in table 2. The results correspond to the inverse relationship between \(\hbar\) and \(\theta\). In turn, the remaining (zero) elements of the first row are found to be of the order of \(10^{-6}\) at worst.

5. Conclusion

In this paper we focus attention on the three-body Coulomb Green’s function operator representation. In particular, we demonstrate numerically, with two simple examples, that use of an appropriate straight-line path of integration provides a non-zero integral representation of the Green’s function operator. We also remark that the potential operator \(\hat{V}\) (13) also contains scalar products \(\hat{r}_{ij} \cdot \hat{k}_i\) with \([ij]\) \(\neq [ls]\) (see, e.g. [13]). Therefore in general the calculation of the the matrix \(\hat{V}\) requires the inversion of transformations (6) which is rather complicated. However, in the case when the momenta \(k_{13}, k_{23}\) and \(k_{12}\) are parallel, the potential (13) matrix elements in the basis (14) can be evaluated analytically. Thus this simple example provides a useful check on the efficiency of the presented numerical scheme. For example, the convergence of the procedure can be tested by enlarging the basis set used to describe the potential (13).

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Appendix A. Matrix representations of one- and two-dimensional operators

A.1. One-dimensional operators

The matrix representation of the operator $\hat{h}_\xi$ (9) in the basis $\{\psi_n(\xi)\}_{n=0}^\infty$ (16), which is orthonormal with respect to $\xi \in [0, \infty)$, is tridiagonal with nonzero elements

\[ h_{n,n}^\xi = b + ik + 2bn, \quad h_{n,n-1}^\xi = (b - ik)n, \quad h_{n,n+1}^\xi = (b + ik)(n + 1). \]  

(A.1)

In addition, the symmetric matrix $Q_\xi$ of the operator $\hat{\xi}$ in the basis (16) is also tridiagonal:

\[ Q_{n,n'} = \begin{cases} -\frac{n}{\theta}, & n' = n - 1, \\ \frac{2n+1}{\theta}, & n' = n, \\ -\frac{n+1}{\theta}, & n' = n + 1. \end{cases} \]  

(A.2)

Hence, the one-dimensional operator $\left[\hat{h}_\xi + 2kt + \mu C\xi\right]$ also has the tridiagonal matrix representation $\left[\hat{h}_\xi + 2kt\hat{I}_\xi + \mu C\hat{Q}_\xi\right]$ ($\hat{I}_\xi$ is the unit matrix) in the basis set (16). Fortunately, the inverse of the matrix $\left[\hat{h}_\xi + 2kt\hat{I}_\xi + \mu C\hat{Q}_\xi\right]$ can be obtained analytically. The elements of the resulting matrix $g^{(\xi)}(\tau)$ are expressed in terms of well-known special functions

\[ g^{(\xi)}_{n_-,n_+}(\tau; \gamma) = \frac{i}{2\gamma} \left( \frac{\zeta - 1}{\zeta} \right) \frac{\theta^{n_+ - n_-}}{\theta^{n_+}} p_n(\tau; \xi) q_n^{(\xi)}(\tau; \xi), \]  

(A.3)

\[ g^{(-\xi)}_{n_-,n_+}(\tau; \gamma) = \frac{i}{2\gamma} \left( \frac{\zeta - 1}{\zeta} \right) \frac{\theta^{n_+ - n_-}}{\theta^{n_+}} p_n(\tau; \xi) \xi^{n_+ + 1} q_n^{(-\xi)}(\tau; \xi), \]  

(A.4)

where $n_-$ is the lesser of $n_1$ and $n_2$, and $n_+$ the greater of the two. Here

\[ \theta = \frac{2b + i(\gamma - k)}{2b - i(\gamma - k)}, \quad \lambda = \frac{2b - i(\gamma + k)}{2b + i(\gamma + k)}, \quad \zeta = \frac{\lambda}{\theta}, \]  

(A.5)

\[ \tau = \frac{k}{\gamma} \left( \frac{\gamma}{2} \right), \]  

(A.6)

\[ \mu C = \frac{k^2}{2} - \mathcal{E}, \quad \mathcal{E} = \frac{\gamma^2}{2}, \]  

(A.7)

and

\[ p_n(\tau; \xi) = (-1)^n \frac{n + \frac{1}{2} - ir}{n!} \left( \frac{1}{2} - ir \right) {}_2F_1 \left( -n, \frac{1}{2} + ir; -n + \frac{1}{2} + ir; \xi \right) \]  

(A.8)

are the polynomials of degree $n$ in $\tau$ which are orthogonal:

\[ \frac{i}{\zeta^m} \left( \frac{\zeta - 1}{\zeta} \right) \int_{-\infty}^{\infty} d\tau \rho(\tau; \xi) p_n(\tau; \xi) p_m(\tau; \xi) = \delta_{nm}, \]  

(A.9)

with respect to the weight function

\[ \rho(\tau; \xi) = \frac{1}{2\pi} \Gamma \left( \frac{1}{2} + ir \right) \Gamma \left( \frac{1}{2} - ir \right) (-\xi)^{-\frac{3}{2}}. \]  

(A.10)

In (A.10) it is considered that $|\arg(-\xi)| < \pi$. The polynomials $p_n$ satisfy the three-term recurrence relation

\[ n\xi p_n(\tau; \xi) + \left[ \frac{2(n + 1)}{2} \right] (\zeta + 1 + ir(\xi - 1)) p_n(\tau; \xi) + (n + 1) p_{n+1}(\tau; \xi) = 0. \]  

(A.11)
The function $q_n^{(\pm)}$ is given by

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

(A.12)

Similarly, the nonzero elements of the tridiagonal matrix $h_{\eta}$ of the operator $\hat{h}_\eta$ (9) in the basis $\{|\eta_(n)(\eta)\rangle\}_{n=0}^{\infty}$ (16) are

$$h_{\eta,n}^\eta = b - ik + 2bn, \quad h_{\eta,n-1}^\eta = (b + ik)n, \quad h_{\eta,n+1}^\eta = (b - ik)(n + 1).$$

(A.13)

Obviously, the nonzero elements of the matrix $Q_\eta$ of the operator $\eta$ in the basis (16) are defined by (A.2). Thus, the elements of the matrix $g^{(\pm)}_\eta$, which is inverse of the matrix $[h_\eta + 2kI_\eta + \mu CQ_\eta]$ ($I_\eta$ is the unit matrix) of the one-dimensional operator $[\hat{h}_\eta + 2k + \mu C]$, are expressed as

$$g_{n_1,n_2}^{(+)}(\tau; \xi) = \frac{i}{2\gamma} \left( \frac{\gamma - 1}{\xi} \right) \frac{\lambda^{n_2-n_1}}{\xi^{n_2}} p_{n_2}(\tau; \xi) q_{n_2}^{(+)}(\tau; \xi),$$

(A.14)

and

$$g_{n_1,n_2}^{(-)(\tau; \xi)} = \frac{i}{2\gamma} \left( \frac{\gamma - 1}{\xi} \right) \frac{\lambda^{n_2-n_1}}{\xi^{n_2}} p_{n_2}(\tau; \xi) q_{n_2}^{(-)}(\tau; \xi).$$

(A.15)

Note that $q_{n}^{(+)}$ ($q_{n}^{(-)}$) are defined in the upper (lower) half of the complex $\gamma$-plane where $|\gamma| > 1$ ($|\gamma| < 1$). $q_{n}^{(+)}$ can be analytically continued onto the lower half-plane by using relation (15.3.7) in [11] for hypergeometric functions, which transforms into the following relationship between $q_{n}^{(+)}$ and $q_{n}^{(-)}$:

$$q_{n}^{(+)}(\tau; \xi) = \xi^{n+1} q_{n}^{(-)}(\tau; \xi) + 2\pi i \rho(\tau; \xi) p_n(\tau; \xi).$$

Then the formulae for the analytical continuations of $g_{n_1,n_2}^{(+)}$ and $g_{n_1,n_2}^{(-)}$ are

$$g_{n_1,n_2}^{(+)}(\tau; \xi) = g_{n_1,n_2}^{(-)}(\tau; \xi) = \frac{\pi}{\gamma} \left( \frac{\xi - 1}{\xi} \right) \frac{\rho^{n_1}}{\lambda^{n_1}} \rho(\tau; \xi) p_{n_1}(\tau; \xi) p_{n_2}(\tau; \xi),$$

(A.17)

and

$$g_{n_1,n_2}^{(-)}(\tau; \xi) = g_{n_1,n_2}^{(+)}(\tau; \xi) = \frac{\pi}{\gamma} \left( \frac{\xi - 1}{\xi} \right) \frac{\rho^{n_2}}{\lambda^{n_2}} \rho(\tau; \xi) p_{n_2}(\tau; \xi) p_{n_2}(\tau; \xi).$$

(A.18)

A.2. Two-dimensional operators

Note first that the completeness relations for eigenfunctions of the one-dimensional operators $[\hat{h}_\xi + 2kI_\xi + \mu C\xi]$ and $[\hat{h}_\eta + 2kI_\eta + \mu C\eta]$ may take the form (see, e.g., [1])

$$\pm \frac{\gamma}{i\tau} \int_{-\infty}^{\infty} d\tau g_{n_1,n_2}^{(+)}(\tau; \xi) = \pm \frac{\gamma}{i\tau} \int_{-\infty}^{\infty} d\tau g_{n_1,n_2}^{(-)}(\tau; \xi) = \frac{1}{2} \delta_{n_1,n_2}.$$  (A.19)

The two-dimensional operator $[\hat{h}_\xi + \hat{h}_\eta + 2k I_\xi + \mu C(\xi + \eta)]$ is also treated analytically within the context of the basis $\{|\phi_{n,m}(\xi, \eta)\rangle\}_{n,m=0}^{\infty}$ (15). In particular, in view of (A.19), the inverse of the infinite matrix

$$[h_\xi \otimes I_\eta + I_\xi \otimes h_\eta + 2k I_\xi \otimes I_\eta + \mu C(I_\xi \otimes I_\eta + I_\xi \otimes Q_\eta)]$$

(A.20)

can be represented in the form of a convolution integral

$$G^{(\pm)}(t_0; \gamma) = \pm \frac{\gamma}{i\tau} \int_{-\infty}^{\infty} d\tau g^{(\pm)}(\tau; \gamma) \otimes g^{(\pm)}(\tau_0 - \tau; \gamma), \quad t_0 = \frac{k}{\gamma} t_0.$$  (A.21)

Finally we note that the matrix representation $G^{(\pm)}$ (A.21) of the two-dimensional Green’s function operator is symmetric in $\xi$ and $\eta$ unlike the corresponding formula obtained in [2].
Appendix B. Calculation of \( G_{n_1, m_1; n_2, m_2}^{(s)} \)

In this appendix we calculate the convolution integrals

\[
G_{n_1, m_1; n_2, m_2}^{(s)}(t_0; \varepsilon) = \frac{\gamma}{4\pi} \int_{-\infty}^{\infty} dt \ g_{n_1, n_2}^{(s)}(\tau; \gamma) \ g_{m_1, m_2}^{(s)}(t_0 - \tau; \gamma). \tag{B.1}
\]

First we use (15.3.5) in [11] to rewrite \( g_{n}^{(s)}(A.12) \) in the form

\[
g_{n_1, n_2}^{(s)}(\tau; \xi) = (-1)^n \left( \frac{\xi}{\xi - 1} \right)^{n+1} \frac{\Gamma(n + 1) \Gamma \left( \frac{1}{2} + i\tau \right)}{\Gamma(n + \frac{1}{2} + i\tau)} \times _2F_1 \left( n + 1, n + 1; n + \frac{3}{2} + i\tau; z \right), \quad z = \frac{1}{1 - \xi}. \tag{B.2}
\]

Then using the integral representation (15.3.1) in [11] of the hypergeometric function, we obtain

\[
g_{n_1, n_2}^{(s)}(\tau; \xi) = \left( \frac{\xi}{1 - \xi} \right)^n \int_0^1 dx \ \frac{e^{i\tau \ln(1-x)} x^n}{\sqrt{1 - x (1 - xz)^{n+1}}}. \tag{B.3}
\]

Thus, equation (A.3) becomes

\[
g_{n_1, n_2}^{(s)}(\tau; \gamma) = \frac{i}{2\gamma} \frac{\theta^{m_2-m_1}}{\xi^{n_2}} \left( \frac{\xi}{1 - \xi} \right)^{m_2} p_{m_1}(\tau; \xi) \int_0^1 dx \ \frac{e^{i\tau \ln(1-x)} x^{m_1}}{\sqrt{1 - x (1 - xz)^{m_1+1}}}. \tag{B.4}
\]

Similarly, we find

\[
g_{m_1, m_2}^{(s)}(t_0 - \tau; \gamma) = \frac{i}{2\gamma} \frac{\lambda^{m_2-m_1}}{\xi^{m_2}} \left( \frac{\xi}{1 - \xi} \right)^{m_2} p_{m_1}(\tau; \xi) \int_0^1 dy \ \frac{e^{i\tau \ln(1-y)} y^{m_1}}{\sqrt{1 - y (1 - yz)^{m_1+1}}}. \tag{B.5}
\]

Inserting the integral representations (B.4) and (B.5) into (B.1) then yields

\[
G_{n_1, m_1; n_2, m_2}^{(s)}(t_0; \varepsilon) = \frac{\gamma}{4\pi} \frac{\theta^{m_2-m_1}}{\lambda^{m_2-m_1}} \left( \frac{\xi}{1 - \xi} \right)^{m_2} \times \int_0^1 dy \ \frac{e^{i\tau \ln(1-y)} y^{m_1}}{\sqrt{1 - y (1 - yz)^{m_1+1}}} \int_0^1 dx \ \frac{e^{i\tau \ln(1-x)} x^{n_1}}{\sqrt{1 - x (1 - xz)^{n_1+1}}} \times \int_{-\infty}^{\infty} dt \ p_{m_1}(\tau; \xi) p_{m_2}(t_0 - \tau; \xi) \ e^{i\tau \ln(1-z)}^\ell. \tag{B.6}
\]

To evaluate (B.6) we note that the integrand contains a polynomial of degree \( n_+ + m_- \) in \( \tau \), and therefore the last integral over \( \tau \) is expressed as a combination of derivatives of the delta function:

\[
\int_{-\infty}^{\infty} dt \ e^{i\tau \ln(1-z)}^\ell = 2\pi (1 - y) \left[ (x - 1) \frac{d}{dx} \right]^\ell \delta(x - y), \quad \ell \leq n_- + m_-, \tag{B.7}
\]

so that

\[
\int_0^1 dy \ \frac{e^{i\tau \ln(1-y)} y^{m_1}}{\sqrt{1 - y (1 - yz)^{m_1+1}}} \int_0^1 dx \ \frac{e^{i\tau \ln(1-x)} x^{n_1}}{\sqrt{1 - x (1 - xz)^{n_1+1}}} \int_{-\infty}^{\infty} dt \ e^{i\tau \ln(1-z)}^\ell, \tag{B.8}
\]

is reduced to

\[
2\pi \int_0^1 dy \ \frac{y^{m_1} (1 - y)^{\frac{1}{2} + \ell} \delta(1 - y)}{(1 - yz)^{m_1+1}} \left[ (1 - y) \frac{d}{dy} \right]^\ell \left( \frac{y^{n_1}}{\sqrt{1 - y (1 - yz)^{n_1+1}}} \right). \tag{B.9}
\]
Clearly, the integral above can be performed in terms of hypergeometric functions. These integrals are most conveniently computed with the help of symbolic algebra software.

In the simplest case $n_1 = m_1 = 0$ one easily obtains

$$G_{\eta_1, \eta_2; 0, 0} (t_0; \mathcal{E}) = \frac{i}{2y} \frac{\theta^m}{\lambda^m} \left( \frac{\zeta}{1 - \zeta} \right) \frac{n^m}{n^m} \int_0^1 dy y^{n+m} (1 - y)^{i t_0} (1 - y \zeta)^{-n-m}$$

$$= \frac{i}{2y} \frac{\theta^m}{\lambda^m} \left( \frac{\zeta}{1 - \zeta} \right) \frac{n^m}{n^m} \frac{\Gamma(n+m+1) \Gamma(1 + i t_0)}{\Gamma(n+m+2 + i t_0)}$$

$$\times \left( \frac{\zeta}{1 - \zeta} \right) \frac{n^m}{n^m} \frac{\Gamma(n+m+1) \Gamma(1 + i t_0)}{\Gamma(n+m+2 + i t_0)}$$

$$\times \left( \frac{\zeta}{1 - \zeta} \right) \frac{n^m}{n^m} \frac{\Gamma(n+m+1) \Gamma(1 + i t_0)}{\Gamma(n+m+2 + i t_0)}$$

$$\times \left( \frac{\zeta}{1 - \zeta} \right) \frac{n^m}{n^m} \frac{\Gamma(n+m+1) \Gamma(1 + i t_0)}{\Gamma(n+m+2 + i t_0)}$$

$$\times \left( \frac{\zeta}{1 - \zeta} \right) \frac{n^m}{n^m} \frac{\Gamma(n+m+1) \Gamma(1 + i t_0)}{\Gamma(n+m+2 + i t_0)}$$

$$\times \left( \frac{\zeta}{1 - \zeta} \right) \frac{n^m}{n^m} \frac{\Gamma(n+m+1) \Gamma(1 + i t_0)}{\Gamma(n+m+2 + i t_0)}$$

$$\times \left( \frac{\zeta}{1 - \zeta} \right) \frac{n^m}{n^m} \frac{\Gamma(n+m+1) \Gamma(1 + i t_0)}{\Gamma(n+m+2 + i t_0)}$$

Matrix elements $G_{\eta_1, \eta_2; \eta_1', \eta_2'}$ with nonzero $n_1$ and $n_2$ ($m_1, m_2 \neq 0$) are also expressed in terms of hypergeometric functions $\left. \frac{\gamma^m}{\lambda^m} \right| \zeta - 1$ with $\ell \geq 1$. Equivalence between (B.1) and (B.6), (B.7), (B.8), (B.9) may be verified numerically.

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