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A parabolic quasi-Sturmian approach to quantum scattering by a Coulomb-like potential

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Abstract A computational method in parabolic coordinates is proposed to treat the scattering of a charged particle from both spherically and axially symmetric Coulomb-like potentials. Specifically, the long-range part of the Hamiltonian is represented in parabolic quasi-Sturmian basis functions, while the short-range part is approximated by a Sturmian L^2-basis-set truncated expansion. We establish an integral representation of the Coulomb Green's function in parabolic coordinates from which we derive a convenient closed form for its matrix elements in the chosen L^2 basis set. From the Green's function, we build quasi-Sturmian functions that are also given in closed form. Taking advantage of their adequate built-in Coulomb asymptotic behavior, scattering amplitudes are extracted as simple analytical sums that can be easily computed. The scheme, based on the proposed quasi-Sturmian approach, proves to be numerically efficient and robust as illustrated with converged results for three different scattering potentials, one of spherical and two of axial symmetry.

1 Introduction

Scattering by central potentials, including spherically symmetric Coulomb-like potentials, can be effectively treated with standard methods using a square-integrable (L^2) basis expressed in spherical coordinates [1]. Scattering by an axially symmetric Coulomb-like potential, on the other hand, is generally less known, it requires more specific mathematical tools and is computationally much more challenging. Meanwhile these types of potentials often arise in molecular physics (e.g., the electron–diatomic-molecule scattering [2–4]) and also are encountered in nuclear (e.g., the proton–deformed-nucleus scattering [5,6]) and atomic physics (e.g., an electron moving in the electrostatic field of an ion in the presence of monochromatic and linearly polarized laser radiation [7]). Mathematically, the axial symmetry can be accounted for by employing a specific coordinate system. For example, the Schrödinger equation for the scattering of a charged particle by two fixed charged centers is known to be separable in spheroidal coordinates (see, e.g., Ref. [8] and references therein). In such a case the solution is represented in the form of a product of radial and angular Coulomb spheroidal functions; the latter are evaluated numerically, not analytically, as eigensolutions

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of the angular equation. The implementation in non-spherical coordinates is seldom applied in practical numerical ab initio calculations since most scattering methods use standard one-center spherical expansions. At the same time, parabolic coordinates (with the $\hat{z}$ axis directed along the symmetry axis if there is one in the considered physical problem) could be an efficient and robust alternative both to the spherical and to the spheroidal coordinates.

In this work we propose a method that makes use of the so-called quasi-Sturmian (QS) basis functions expressed in closed form in parabolic coordinates, similar to those derived in spherical coordinates [9]. Our parabolic QS approach is capable of treating efficiently quantum scattering problems not only in the two-center Coulomb case but in the general case of an axially symmetric Coulomb-like potential. Moreover, as demonstrated below, the approach has a much larger outreach since it can be successfully applied also to scattering on central Coulomb-like potentials.

Expansions of the Coulomb wave functions in a complete set of square integrable (L^2) parabolic Sturmians were considered in Ref. [10]. Specifically, the regular and irregular solutions in this basis set were obtained in analytic form. As mentioned above, here we develop the scattering formulation making use of parabolic QS basis functions. These are generated by applying an appropriate Coulomb Green's operator to the parabolic Sturmians multiplied by their weight. Consequently, the resulting QS basis functions satisfy the appropriate Coulomb boundary conditions and an expansion of the scattering solution for Coulomb-like potentials is anticipated to be convergent in the entire space. In order to solve a scattering problem with a Coulomb plus short-range potential of spherical or axial symmetry, we express the wave function as $\psi^{(\pm)} = \psi_{\rm C}^{(\pm)} + \psi_{\rm sc}^{(\pm)}$, where $\psi_{\rm C}^{(\pm)}$ is a Coulomb wave function. The scattering Schrödinger equation is then recast into a driven equation for the unknown $\psi_{\rm sc}^{(\pm)}$ with a square-integrable inhomogeneous term. We further propose to find the solution, subject to outgoing or incoming boundary conditions, with an expansion of $\psi_{\rm sc}^{(\pm)}$ in terms of parabolic QS functions. It should be noted that we have already used such an approach to calculate the outgoing electron states in laser-assisted $(e, 2e)$ processes on atomic hydrogen [11,12]. The purpose of the present paper is twofold. First, we wish to present the formulation of the proposed parabolic approach by (i) giving a detailed derivation of the Coulomb Green's function representation in the Sturmian basis, (ii) analyzing the asymptotic behavior of the parabolic QS functions in detail, and (iii) showing how one can readily extract from it the amplitude for potential scattering. The second purpose is to demonstrate that the proposed scheme is computationally efficient and robust, and able to deal with a variety of potentials—with either axial or spherical symmetry—that may occur in nuclear, atomic or molecular physics.

The remainder of this paper is as follows. In Sect. 2 we focus on the Coulomb Green's function matrix representation in the parabolic Sturmian basis. Specifically, we express the matrix elements in closed form in terms of hypergeometric functions. Section 3 provides an integral representation of the parabolic QS functions, from which we deduce their leading asymptotic behavior. This result allows us to express the scattering amplitude in terms of the coefficients derived from the expansion of the solution $\psi_{\rm sc}^{(\pm)}$ on the basis of parabolic QS functions. In Sect. 4, the numerical efficiency of the parabolic QS basis set is illustrated with applications to the scattering of an electron by (i) a Coulomb plus spherically symmetric short-range potential, (ii) a Coulomb potential dressed by a high-frequency linearly polarized laser field, and (iii) a two-center Coulomb potential. Finally, Sect. 5 provides a summary of this work.

Atomic units ($\hbar = m_e = e = 1$) are assumed throughout.

2 Coulomb Green's function

Consider the two-particle Coulomb Hamiltonian in the center-of-mass reference frame,

$$\hat{H}_{\mathrm{C}} = -\frac{1}{2\mu}\Delta - \frac{Z}{r}, \tag{1}$$

for an electron and a nucleus of charge Z and a reduced mass μ. The kernels $G^{(\pm)}\left(k; \mathbf{r}, \mathbf{r}'\right)$ of the corresponding Green's operators $\hat{G}^{(\pm)} = (\hat{H}_{\mathrm{C}} - E)^{-1}$ satisfy the equation

$$\left(H_{\mathrm{C}} - \frac{k^2}{2\mu}\right) G^{(\pm)}\left(k; \mathbf{r}, \mathbf{r}'\right) = \delta(\mathbf{r} - \mathbf{r}'), \tag{2}$$

where the energy is $E = k^2/(2\mu)$; the symbol (+) or (−) corresponds to an outgoing wave or an incoming wave, respectively. In terms of the parabolic coordinates $\xi \in [0, \infty[$, $\eta \in [0, \infty[$ and $\phi \in [0, 2\pi[$, the Cartesian coordinates are defined by $x = \sqrt{\xi\eta}\cos\phi$, $y = \sqrt{\xi\eta}\sin\phi$ and $z = (\xi - \eta)/2$; conversely, we have $\xi = r + z$, $\eta = r - z$ and $\phi = \tan^{-1}(y/x)$ where $r = \sqrt{x^2 + y^2 + z^2}$ is the distance from the origin. In such parabolic coordinates, the Green's function can be represented by the expansion

$$G^{(\pm)}\left(k; \mathbf{r}, \mathbf{r}'\right) = \frac{1}{2\pi}\sum_{m=-\infty}^{\infty} \mathrm{e}^{im(\phi-\phi')}\mathcal{G}^{|m|(\pm)}\left(k; \xi, \eta; \xi', \eta'\right). \tag{3}$$

The partial components $\mathcal{G}^{|m|(\pm)}$ obey the equation

$$\frac{1}{2\mu}\,\hat{h}\,\mathcal{G}^{|m|(\pm)}(k;\ \xi, \eta;\ \xi', \eta') = \delta(\xi - \xi')\delta(\eta - \eta'), \tag{4}$$

where

$$\hat{h} = -\left(\frac{\partial}{\partial\xi}\,\xi\,\frac{\partial}{\partial\xi} + \frac{\partial}{\partial\eta}\,\eta\,\frac{\partial}{\partial\eta}\right) + k\beta + \frac{m^2}{4\xi} + \frac{m^2}{4\eta} - (\xi + \eta)\frac{k^2}{4}, \tag{5}$$

and $\beta = -\mu Z/k$.

2.1 An integral representation of the Coulomb Green's function

The operator $\hat{h}$ can be split into the sum

$$\hat{h} \equiv \hat{h}_{\xi,\,\tau} + \hat{h}_{\eta,\,\beta-\tau}, \tag{6}$$

where

$$\hat{h}_{x,\,t} \equiv -\frac{\partial}{\partial x}x\frac{\partial}{\partial x} + kt + \frac{\lambda^2}{4x} - \frac{k^2}{4}x, \tag{7}$$

with τ playing the role of a charge separating parameter. Then, in order to obtain a kernel representing the inverse operator $\hat{h}^{-1}$, we make use of the linearly independent solutions of the equation

$$\hat{h}_{x,\,t}\,f(x, t) = 0, \tag{8}$$

namely

$$\begin{aligned} u(x,t) &= \mathrm{e}^{i\frac{k}{2}x}\,(-ikx)^{\frac{\lambda}{2}}\,M\left(\frac{1+\lambda}{2}+it,\ 1+\lambda;\ -ikx\right) \\ &= \mathrm{e}^{-i\frac{k}{2}x}\,(-ikx)^{\frac{\lambda}{2}}\,M\left(\frac{1+\lambda}{2}-it,\ 1+\lambda;\ ikx\right), \\ w^{(\pm)}(x,t) &= \mathrm{e}^{\pm i\frac{k}{2}x}\,(\mp ikx)^{\frac{\lambda}{2}}\,U\left(\frac{1+\lambda}{2}\pm it,\ 1+\lambda;\ \mp ikx\right), \end{aligned} \tag{9}$$

where M and U are the Kummer functions of, respectively, first and second kind [13]. The corresponding one-dimensional Green's functions $g^{(\pm)}$, defined through

$$\hat{h}_{x,t}\,g^{(\pm)}(t;\ x,x') = \delta(x-x'), \tag{10}$$

satisfy the condition

$$\left[-x\frac{\partial}{\partial x}g^{(\pm)}(t;\ x,x')\right]_{x'-\varepsilon}^{x'+\varepsilon} = 1 \tag{11}$$

for small ε. A standard representation is given by [14]

$$g^{(\pm)}(t;\ x,x') = -\frac{u(x_<,\ t)\,w^{(\pm)}(x_>,t)}{x'\,W\left(u,\ w^{(\pm)}\right)}, \tag{12}$$

with $x_< = \min(x,x')$, $x_> = \max(x,x')$ and

$$W\left(u,\ w^{(\pm)}\right) \equiv u(x',\ t)\frac{d}{dx'}\left(w^{(\pm)}(x',t)\right) - \frac{d}{dx'}\left(u(x',\ t)\right)w^{(\pm)}(x',t). \tag{13}$$

Then, making use of the Wronskian of the Kummer functions (Eq. (13.1.22) in Ref. [13]), we find

$$g^{(\pm)}(t;\ x,x') = \frac{\Gamma\left(\frac{1+\lambda}{2}\pm it\right)}{\Gamma(1+\lambda)}\frac{1}{(\mp ikx_<)^{\frac{1}{2}}}\mathcal{M}_{\mp it,\frac{\lambda}{2}}(\mp ikx_<)\frac{1}{(\mp ikx_>)^{\frac{1}{2}}}\mathcal{W}_{\mp it,\frac{\lambda}{2}}(\mp ikx_>), \tag{14}$$

where $\mathcal{M}$ and $\mathcal{W}$ are the Whittaker functions [13]. Finally, using the integral representation of the product of Whittaker functions (see, e.g., Ref. [15], p. 86, Eq. (5b); Ref. [16], p. 742, Eq. (6.669, 1)) we have

$$g^{(\pm)}(t;\ x,x') = \int_0^\infty \mathrm{d}z\,\exp\left\{\pm i\frac{k}{2}(x+x')\cosh z\right\}\left(\coth\frac{z}{2}\right)^{\mp 2it} I_\lambda\left(\mp ik\sqrt{xx'}\sinh z\right), \tag{15}$$

where I_λ is the modified Bessel function [13].

The two-dimensional Green's function for the operator $\hat{h}$ (6) is then obtained as a convolution integral over the charge separating parameter τ:

$$\pm\frac{k}{2\pi i}\int_{-\infty}^{\infty}\mathrm{d}\tau\,g^{(\pm)}(\tau;\ \xi,\ \xi')\,g^{(\pm)}(\beta-\tau;\ \eta,\ \eta'). \tag{16}$$

Thus, inserting (15) into (16) and integrating over τ, we obtain the following expression for $\mathcal{G}^{\lambda(\pm)}$:

$$\mathcal{G}^{\lambda(\pm)}(k;\ \xi,\eta;\ \xi',\eta') = \mp i\mu k \int_0^\infty \mathrm{d}z\ \sinh z \left(\coth\frac{z}{2}\right)^{\mp 2i\beta} \mathrm{e}^{\pm i\frac{k}{2}(\xi+\xi'+\eta+\eta')\cosh z} \times I_\lambda\left(\mp ik\sqrt{\xi\xi'}\sinh z\right) I_\lambda\left(\mp ik\sqrt{\eta\eta'}\sinh z\right). \tag{17}$$

This integral representation of the Coulomb Green's function slightly differs from that given in Ref. [17] (see also Refs. [18,19]).

2.2 Matrix elements of the Green's function in the Sturmian basis

Consider the basis of Sturmian functions

$$|n_1 n_2 m\rangle = \frac{\mathrm{e}^{im\phi}}{\sqrt{2\pi}}\,\varphi_{n_1}^{|m|}(\xi)\,\varphi_{n_2}^{|m|}(\eta), \tag{18}$$

where the square-integrable functions $\varphi_n^{|m|}$ are defined in terms of the associated Laguerre polynomials $L_n^{|m|}$ [13]:

$$\varphi_n^{|m|}(\rho) = \sqrt{\frac{2b\Gamma(n+1)}{\Gamma(n+1+|m|)}}\,(2b\rho)^{|m|/2}\mathrm{e}^{-b\rho}L_n^{|m|}(2b\rho), \tag{19}$$

with the basis scale parameter b. The basis functions (18) obey the following orthonormalization condition:

$$\langle n_1 n_2 m|\frac{4}{(\xi+\eta)}|n_1' n_2' m'\rangle = \delta_{n_1 n_1'}\delta_{n_2 n_2'}\delta_{mm'}. \tag{20}$$

Next, we define the functions

$$|\widetilde{n_1 n_2 m}\rangle = \frac{4}{(\xi+\eta)}|n_1 n_2 m\rangle \tag{21}$$

which represent the orthogonal complements to (18).

In this $|\widetilde{n_1 n_2 m}\rangle$ representation, the matrix elements of the Green's function are given by

$$\left[G^{(\pm)}\right]^n_{n_1 n_2 m;\, n_1' n_2' m'} \equiv \delta_{m'm}\mathcal{G}^{|m|(\pm)}_{n_1' n_2';\, n_1 n_2}(\beta_n, k_n), \tag{22}$$

where

$$\begin{aligned}\mathcal{G}^{|m|(\pm)}_{n_1' n_2';\, n_1 n_2}(\beta,k) &\equiv \langle\widetilde{n_1' n_2' m}|\hat{G}^{(\pm)}|\widetilde{n_1 n_2 m}\rangle \\ &= \int_0^\infty \mathrm{d}\xi \int_0^\infty \mathrm{d}\eta \int_0^\infty \mathrm{d}\xi' \int_0^\infty \mathrm{d}\eta' \\ &\quad \varphi_{n_1'}^{|m|}(\xi)\varphi_{n_2'}^{|m|}(\eta)\,\mathcal{G}^{|m|(\pm)}(k;\xi,\eta;\xi',\eta')\varphi_{n_1}^{|m|}(\xi')\varphi_{n_2}^{|m|}(\eta').\end{aligned} \tag{23}$$

In Appendix A we show how such four-dimensional integrals can be calculated step by step. We found it computationally convenient to express the matrix elements as the finite sum

$$\mathcal{G}^{\lambda(+)}_{n_1' n_2';\, n_1 n_2}(\beta,k) = \frac{2i\mu}{k}(1-\zeta^2)(-\zeta)^K \sqrt{\binom{n_1'+\lambda}{n_1'}\binom{n_2'+\lambda}{n_2'}\binom{n_1+\lambda}{n_1}\binom{n_2+\lambda}{n_2}}$$

$$\times \sum_{\ell=0}^{u+v} c_\ell \, \zeta^{-2\ell} \, \frac{\Gamma(\lambda+\ell+1+i\beta)\Gamma(K+1-2\ell)}{\Gamma(K+\lambda+2-\ell+i\beta)}$$
$$\times {}_2F_1\left(K-2\ell+1, -\lambda-\ell+i\beta; K+\lambda+2-\ell+i\beta; \zeta^2\right), \quad (24)$$

where ${}_2F_1$ is the Gauss hypergeometric function [13], $K = n_1' + n_2' + n_1 + n_2$, $u = \min(n_1, n_1')$, $v = \min(n_2, n_2')$, and

$$\zeta = \frac{b + i\frac{k}{2}}{b - i\frac{k}{2}}. \quad (25)$$

The matrix elements of $\mathcal{G}^{\lambda(-)}$ (for real positive k) are simply the complex conjugates of those of $\mathcal{G}^{\lambda(+)}$. We have found that in order to satisfy Eq. (2) (to within 10^{-15}) in the matrix representation, the arbitrary precision arithmetic libraries gmp, mpfr and mpc should be applied. Note that an alternative expansion of the Green' function kernel in terms of the Laguerre basis functions of imaginary arguments has been suggested in Ref. [19]; while very interesting, such an expansion converges very slowly and for this reason is not suitable for the computation of Green's function matrix elements.

3 Quasi-Sturmian functions in parabolic coordinates

In parabolic coordinates, the quasi-Sturmian functions subject to appropriate boundary conditions are defined in Ref. [9] through the Green's operator $\hat{G}^{(\pm)}$, namely

$$Q^{(\pm)}_{n_1 n_2 m}(k;\xi,\eta,\phi) = \hat{G}^{(\pm)} \widetilde{|n_1 n_2 m\rangle}. \quad (26)$$

Let us separate the ϕ dependence,

$$Q^{(\pm)}_{n_1 n_2 m}(k;\xi,\eta,\phi) = \frac{\mathrm{e}^{im\phi}}{\sqrt{2\pi}} \mathcal{P}^{|m|(\pm)}_{n_1 n_2}(k;\xi,\eta), \quad (27)$$

and consider the "radial" part $\mathcal{P}^{\lambda(\pm)}$ which, in view of (26), (21) and (18), is expressed in the form

$$\mathcal{P}^{\lambda(\pm)}_{n_1 n_2}(k;\xi,\eta) = \int_0^\infty \mathrm{d}\xi' \int_0^\infty \mathrm{d}\eta' \, \mathcal{G}^{\lambda(\pm)}(k;\ \xi,\eta;\ \xi',\eta') \varphi^\lambda_{n_1}(\xi') \varphi^\lambda_{n_2}(\eta'). \quad (28)$$

To evaluate it we insert the integral representation (17) of the Green's function, interchange the integration order, and integrate first over ξ' and η' with the help of the expression in Ref. [20] (p. 474, Eq. (12.19.2, 6)) for the integral

$$\int_0^\infty \mathrm{d}x x^\lambda \mathrm{e}^{-px} I_\lambda(b\sqrt{x}) L^\lambda_n(cx). \quad (29)$$

Substituting $z \to s = \left(\tanh\frac{\xi}{2}\right)^2$ in the resulting integral, one obtains

$$\mathcal{P}^{\lambda(\pm)}_{n_1 n_2}(k;\xi,\eta) = 2\mu(1+\zeta^{\pm 1}) \sqrt{\frac{n_1! n_2!}{(n_1+\lambda)!(n_2+\lambda)!}} \left(2b\sqrt{\xi\eta}\right)^\lambda \mathrm{e}^{-b(\xi+\eta)}$$

$$\times \int_0^1 \mathrm{d}s\,(1-s)^{\pm i\beta+\lambda}\left(1-\zeta^{\pm 1}s\right)^{\mp i\beta+\lambda}\left(1-s-\zeta^{\pm 1}s\right)^{n_1+n_2}$$
$$\times \exp\left[2b(\xi+\eta)\frac{\zeta^{\pm 1}s}{(1+\zeta^{\pm 1})}\right]$$
$$\times L_{n_1}^{\lambda}\left(2b\xi\frac{(1-s)(1-\zeta^{\pm 1}s)}{(1-s-\zeta^{\pm 1}s)}\right)L_{n_2}^{\lambda}\left(2b\eta\frac{(1-s)(1-\zeta^{\pm 1}s)}{(1-s-\zeta^{\pm 1}s)}\right). \quad (30)$$

This integral representation allows us to explore the asymptotic behavior of the QS functions, for large distances r, i.e., for large $(\xi+\eta)/2$. Using the fact that $\sqrt{\xi\eta}=\sqrt{x^2+y^2}=r\sin\theta=(1/2)(\xi+\eta)\sin\theta$, we obtain (see details in Appendix B)

$$\mathcal{P}_{n_1n_2}^{\lambda(+)}(k;\xi,\eta)\underset{r\to\infty}{\longrightarrow}\mathcal{A}_{n_1n_2}^{\lambda(+)}(\theta)\,\frac{\exp\{i\,[kr-\beta\ln(2kr)]\}}{r}, \quad (31)$$

where the amplitudes $\mathcal{A}_{n_1n_2}^{\lambda(+)}$ are expressed as

$$\mathcal{A}_{n_1n_2}^{\lambda(+)}(\theta)=\frac{i\mu}{k}\sqrt{\frac{n_1!n_2!}{(n_1+\lambda)!(n_2+\lambda)!}}\,\zeta^{-i\beta}\mathrm{e}^{-\frac{\pi\beta}{2}}\left(\frac{1}{\zeta}-\zeta\right)^{\lambda+1}\left(\frac{\sin\theta}{2}\right)^{\lambda}(-\zeta)^{n_1+n_2}$$
$$\times\sum_{\nu_1=0}^{n_1}\sum_{\nu_2=0}^{n_2}c_{\nu_1}^{(n_1,\lambda)}c_{\nu_2}^{(n_2,\lambda)}$$
$$\times\Gamma(i\beta+\lambda+\nu_1+\nu_2+1)(1-\zeta^{-2})^{\nu_1+\nu_2}\left(\cos\frac{\theta}{2}\right)^{2\nu_1}\left(\sin\frac{\theta}{2}\right)^{2\nu_2}, \quad (32)$$

with the coefficients $c_\nu^{(n,\lambda)}$ defined by [13]

$$c_\nu^{(n,\lambda)}=(-1)^\nu\frac{(n+\lambda)!}{(n-\nu)!(\nu+\lambda)!\nu!}. \quad (33)$$

We have therefore obtained the desired result: the parabolic QS functions (26) possess the leading asymptotic behavior given by

$$\mathcal{Q}_{n_1n_2m}^{(\pm)}(k;\xi,\eta,\phi)\underset{r\to\infty}{\longrightarrow}\frac{\mathrm{e}^{im\phi}}{\sqrt{2\pi}}\mathcal{A}_{n_1n_2}^{|m|(\pm)}(\theta)\,\frac{\exp\{\pm\,i\,[kr-\beta\ln(2kr)]\}}{r}, \quad (34)$$

with

$$\mathcal{A}_{n_1n_2}^{\lambda(-)}(\theta)=\left[\mathcal{A}_{n_1n_2}^{\lambda(+)}(\theta)\right]^*. \quad (35)$$

4 Application to potential scattering

We consider below, using our parabolic QS approach, the scattering of a particle of energy $E=k^2/(2\mu)$ from three different potentials of the form

$$V(\mathbf{r})=-\frac{Z}{r}+U(\mathbf{r}), \quad (36)$$

where $U(\mathbf{r})$ is a short-range potential of either spherical or axial symmetry. Selecting outgoing boundary conditions, we wish to solve the Schrödinger equation

$$[H_\mathrm{C}+U(\mathbf{r})-E]\,\psi^{(+)}(\mathbf{r})=0. \quad (37)$$

Using the standard ansatz

$$\psi^{(+)}(\mathbf{r}) = \psi_{\mathrm{C}}^{(+)}(\mathbf{r}) + \psi_{\mathrm{sc}}(\mathbf{r}), \tag{38}$$

where $\psi_{\mathrm{C}}^{(+)}$ is the Coulomb wave [21]

$$\psi_{\mathrm{C}}^{(+)}(\mathbf{r}) = \frac{1}{(2\pi)^{3/2}}\, \mathrm{e}^{-\frac{1}{2}\pi\beta}\, \Gamma(1+i\beta)\mathrm{e}^{i\mathbf{kr}}\, {}_1F_1(-i\beta, 1; i(kr - \mathbf{kr})), \tag{39}$$

Eq. (37) is transformed into a driven equation for the scattering function ψ_{sc}:

$$[H_{\mathrm{C}} + U(\mathbf{r}) - E]\, \psi_{\mathrm{sc}}(\mathbf{r}) = -U(\mathbf{r})\psi_{\mathrm{C}}^{(+)}(\mathbf{r}). \tag{40}$$

We propose to solve it by expanding ψ_{sc} in terms of $N \times N$ parabolic QS basis functions (hereafter we restrict ourselves to the case with only one symmetry axis, which is defined by the incident momentum $\mathbf{k}$):

$$\psi_{\mathrm{sc}}(\mathbf{r}) = \sum_{n_1,n_2=0}^{N-1} C_{n_1,n_2}\, Q^{(+)}_{n_1 n_2 0}(k; \xi, \eta, \phi). \tag{41}$$

Inserting (41) into (40) gives, in view of the definition (26),

$$\sum_{n_1',n_2'=0}^{N-1} \left[\hat{I} + \hat{U}\hat{G}^{(+)}\right] C_{n_1',n_2'} \widetilde{|n_1' n_2' 0\rangle} = -U(\mathbf{r})\psi_{\mathrm{C}}^{(+)}(\mathbf{r}). \tag{42}$$

Then, projecting (42) onto $\langle n_1 n_2 0|$ and inserting the unit operator

$$\hat{I} = \sum_{q_1,q_2,m} |q_1 q_2 m\rangle\widetilde{\langle q_1 q_2 m|}\, \tag{43}$$

between $\hat{U}$ and $\hat{G}^{(+)}$, we obtain the algebraic equation for the coefficients $C_{n_1',n_2'}$:

$$\sum_{n_1',n_2'=0}^{N-1} \left[\delta_{n_1,n_1'}\delta_{n_2,n_2'} + \sum_{q_1,q_2} \mathcal{U}_{n_1 n_2;\, q_1 q_2}\, \mathcal{G}^{0(+)}_{q_1 q_2;\, n_1' n_2'}(\beta, k)\right] C_{n_1',n_2'} = -d_{n_1,n_2}, \tag{44}$$

where

$$\mathcal{U}_{n_1 n_2;\, n_1' n_2'} = \langle n_1 n_2 0|\hat{U}|n_1' n_2' 0\rangle, \tag{45}$$

$$d_{n_1,n_2} = \langle n_1 n_2 0|\hat{U}|\psi_{\mathrm{C}}^{(+)}\rangle. \tag{46}$$

The matrix elements (45) of the short-range potential as well as the components (46) of the right-hand side vector are evaluated numerically. In doing this, we approximate the two-dimensional integrals by the n-point Gauss-Laguerre quadrature formula [13], and we take $n = 256$. In order to compute all the needed elements for the matrix equation in a reasonable amount of time we use GPU (CUDA parallel programming model). The matrix equation (44) is solved using the EESL library linear algebra subroutine zgesv.

The basis scale parameter $b > 0$ in Eq. (19) can be chosen freely. As a thumb rule, the following general prescription in terms of the length parameter b^{-1} can be formulated: the short-range potential should change appreciably on this length, but the latter should not exceed the characteristic range of the potential. In the present investigation we chose, for a given potential, a value of b which seemed reasonable and provided a satisfactory numerical convergence. In a more refined approach, one could envisage searching for an optimal choice

of b that would minimize the size of the matrix representation (45) to obtain a desired convergence rate.

According to the two-potential formula (see, e.g., Ref. [22]), the scattering amplitude can be presented as

$$f(\theta) = f_{\mathrm{C}}(\theta) + \tilde{f}(\theta), \tag{47}$$

where

$$f_{\mathrm{C}}(\theta) = -\frac{\beta}{2k}\frac{\Gamma(1+i\beta)}{\Gamma(1-i\beta)}\frac{\exp\left(-i\beta\ln\left[\sin\frac{\theta}{2}\right]^2\right)}{\left[\sin\frac{\theta}{2}\right]^2} \tag{48}$$

is the Coulomb amplitude. The amplitude $\tilde{f}(\theta)$ contains the effect of the short-range potential $U(\mathbf{r})$. From the asymptotic behavior of the QS function (34) and of the Coulomb wave (39), one finds that it is expressed in terms of the coefficients C_{n_1,n_2} as

$$\tilde{f}^N(\theta) = 2\pi \sum_{n_1,n_2=0}^{N-1} C_{n_1,n_2}\mathcal{A}^{0(+)}_{n_1n_2}(\theta). \tag{49}$$

First, we illustrate the efficiency of our approach in the case of a central potential given by a Coulomb plus Yukawa potential. Then, we provide illustrations for two non-central axially symmetric potentials: one arises in the accelerated Kramers–Henneberger frame when treating the electron scattering on a Coulomb potential in the presence of a linearly polarized laser field in the high-frequency limit, and the other is generated by two Coulomb centers as, for example, two nuclei in a homonuclear diatomic molecule.

4.1 Scattering by a Coulomb plus Yukawa potential

Let the particle, say an electron, be submitted to the central potential of the form (36) with a Yukawa potential

$$U(r) = U_0\frac{\mathrm{e}^{-2ar}}{r}. \tag{50}$$

The matrix elements (45) and (46) for this potential are given by

$$\mathcal{U}_{n_1n_2;\,n_1'n_2'} = \frac{U_0}{2}\left(\frac{2b}{2b+a}\right)^2\left(\frac{a}{2b+a}\right)^{n_1+n_2+n_1'+n_2'} \times {}_2F_1\left(-n_1,-n_1';1;\left(\frac{2b}{a}\right)^2\right){}_2F_1\left(-n_2,-n_2';1;\left(\frac{2b}{a}\right)^2\right), \tag{51}$$

$$d_{n_1,n_2} = \frac{U_0}{2}\frac{2b}{\left((a+b)^2+\frac{k^2}{4}\right)}\frac{1}{2\pi}\mathrm{e}^{-\frac{\beta\pi}{2}}\Gamma(1+i\beta)$$
$$\times\left(\frac{a+b-i\frac{k}{2}}{a+b-i\frac{k}{2}}\right)^{i\beta}\left(\frac{a-b-i\frac{k}{2}}{a+b-i\frac{k}{2}}\right)^{n_1}\left(\frac{a-b+i\frac{k}{2}}{a+b+i\frac{k}{2}}\right)^{n_2}$$
$$\times\,{}_2F_1\left(-n_2,-i\beta;1;\frac{2ikb}{(a-b+i\frac{k}{2})(a+b-i\frac{k}{2})}\right). \tag{52}$$

In order to suppress the Gibbs oscillations associated with the use of finite expansions, we follow Papp's proposal [1] and employ the σ factors

$$\sigma_n^N = \frac{1-\exp\left\{-[\alpha(n-N-1)/(N+1)]^2\right\}}{1-\exp(-\alpha^2)}, \quad \alpha = 6. \tag{53}$$

Specifically, we replace $\mathcal{U}_{n_1n_2;\,n_1'n_2'}$ in (44) by $\sigma_{n_1}^N\sigma_{n_2}^N\mathcal{U}_{n_1n_2;\,n_1'n_2'}$. The use of the smoothing factors allows us to improve considerably the rate of convergence in the case of short-range potentials. On the other hand, for the slowly decaying potentials considered in the next subsections we have found that these factors do not have such an effect.

The amplitude $\tilde{f}(\theta)$ can be presented in terms of the partial-wave expansion [22,23]:

$$\tilde{f}(\theta) = \frac{1}{2ik}\sum_{\ell=0}^{\infty}(2\ell+1)\,\mathrm{e}^{2i\sigma_\ell}\left(\mathrm{e}^{2i\delta_\ell}-1\right)P_\ell(\cos\theta), \tag{54}$$

where $\sigma_\ell = \mathrm{Arg}\,[\Gamma(\ell+1+\mathrm{i}\beta)]$ is the Coulomb phase shift. According to Eq. (49), the ℓ-wave phase shift δ_ℓ is determined by

$$\mathrm{e}^{2i\delta_\ell^N} = 1+2\pi ik\mathrm{e}^{-2i\sigma_\ell}\sum_{n_1,n_2=0}^{N-1}C_{n_1,n_2}\int_0^\pi \mathcal{A}_{n_1n_2}^{0(+)}(\theta)P_\ell(\cos\theta)\sin\theta\mathrm{d}\theta. \tag{55}$$

The angular integration does not present difficulties in view of the $\mathcal{A}_{n_1n_2}^{0(+)}(\theta)$ amplitude's form (32). Since here $\lambda = 0$, the angular part is given by

$$\left(\cos\frac{\theta}{2}\right)^{2\nu_1}\left(\sin\frac{\theta}{2}\right)^{2\nu_2}, \tag{56}$$

and one thus needs the integrals

$$\int_{-1}^{1}\left(\frac{1+x}{2}\right)^{\nu_1}\left(\frac{1-x}{2}\right)^{\nu_2}P_\ell(x)\mathrm{d}x. \tag{57}$$

For the s-wave, $\ell = 0$, we have

$$I_{n,m} = \int_{-1}^{1}\left(\frac{1+x}{2}\right)^n\left(\frac{1-x}{2}\right)^m\mathrm{d}x = 2B(n+1,m+1) = 2\frac{\Gamma(n+1)\Gamma(m+1)}{\Gamma(n+m+2)} \tag{58}$$

and for the p-wave, $\ell = 1$,

$$\int_{-1}^{1}\left(\frac{1+x}{2}\right)^n\left(\frac{1-x}{2}\right)^m P_1(x)\mathrm{d}x = I_{n+1,m} - I_{n,m+1}. \tag{59}$$

Table 1 Convergence of the phase shifts δ_0 and δ_1 for the potential $V(r) = -\frac{2}{r} + 4\frac{\exp(-2r)}{r}$ with $k = \sqrt{2E} = 0.5$ as a function of the size N of the parabolic QS basis set

N	$\lvert\gamma_{0,N}\rvert$	$\delta_0(k)$	$\lvert\gamma_{1,N}\rvert$	$\delta_1(k)$
5	0.9891837	1.361369	1.002327	−0.5604802
6	0.9970151	1.362364	0.9948140	−0.5513566
7	0.9982502	1.364919	0.9950018	−0.5546755
8	0.9982024	1.364175	1.000458	−0.5547838
9	0.9997361	1.364197	0.9998475	−0.5544229
10	0.9998452	1.364368	0.9994945	−0.5550903
11	0.9997685	1.364291	1.000024	−0.5553326
12	0.9999001	1.364218	1.000183	−0.5552601
13	0.9999905	1.3642245	1.000011	−0.5552594
14	0.9999871	1.364237	0.9999374	−0.5553244
15	0.9999683	1.364230	0.9999871	−0.5553654
16	0.9999756	1.364218	1.000030	−0.5553599
17	0.9999926	1.364215	1.000017	−0.5553473
18	0.9999989	1.364219	0.9999887	−0.5553522
19	0.9999945	1.364221	0.9999851	−0.5553655
20	0.9999915	1.364218	0.9999999	−0.5553708
21	0.9999944	1.364216	1.000008	−0.5553673
22	0.9999986	1.364216	1.000003	−0.5553642
23	0.9999995	1.364217	0.9999950	−0.5553661
24	0.9999979	1.364218	0.9999949	−0.5553701
25	0.9999970	1.364217	1.000000	−0.5553716

In Table 1 the phase shifts δ_0^N and δ_1^N are shown for the same parameters as in Ref. [1]: $Z = 2$, $U_0 = 4$, $a = 2$, $k = 0.5$. In our calculations we set the basis scale parameter $b = 1$ in (19). It is clear that the convergence with increasing N is rapidly achieved. The calculated modulus of $\gamma_{\ell,N} = \mathrm{e}^{2i\delta_\ell^N}$ is also seen to approach the exact value, i.e., unity.

Obviously, solving the scattering problem with a central potential such as (50) can be easily achieved with standard methods that use the natural and efficient choice of spherical coordinates. The purpose of this first illustration was to numerically demonstrate that our parabolic approach can also deal satisfactorily with central potentials and is not restricted to potentials with axial symmetry as in the next two illustrations.

4.2 Electron scattering by a Coulomb potential in the presence of an intense high-frequency laser field

In this second example we consider a short-range noncentral potential U of the form

$$U(\mathbf{r}) = V_0(\mathbf{a}_0; \mathbf{r}) + \frac{Z}{r}, \tag{60}$$

where V_0 is a "dressed" Coulomb potential [24,25]. The latter arises within the Floquet theory as applied to the Schrödinger equation in the Kramers–Henneberger representation for an one-electron atom in a laser field described by the vector potential $\mathbf{A}(t) = \mathbf{A}_0 \cos(\omega t)$,

where ω is the laser frequency. In the Kramers–Henneberger frame [7] we have to deal with the space-translated Coulomb potential

$$V[\mathbf{r}+\mathbf{a}(t)] = -\frac{Z}{|\mathbf{r}+\mathbf{a}(t)|}, \tag{61}$$

where

$$\mathbf{a}(t) = \frac{1}{c}\int_{-\infty}^{t} \mathbf{A}(\tau)\mathrm{d}\tau = \mathbf{a}_0 \sin(\omega t) \tag{62}$$

is the displacement vector, with $\mathbf{a}_0 = \mathbf{A}_0/(\omega c)$ directed along the z axis and representing the so-called quiver amplitude. In the high-frequency limit, such a potential is approximated by its zeroth Fourier component [24,25]

$$V_0(\mathbf{a}_0;\mathbf{r}) = -\frac{2Z}{\pi}(r_+ r_-)^{-\frac{1}{2}} K\left(\left[\frac{1-\hat{\mathbf{r}}_+\cdot\hat{\mathbf{r}}_-}{2}\right]^{\frac{1}{2}}\right), \tag{63}$$

where $\mathbf{r}_\pm = \mathbf{r} \pm \mathbf{a}_0$ and K is a complete elliptic integral of the first kind [13].

In the numerical implementation of our parabolic QS approach we choose the incident wave vector $\mathbf{k}$ to be parallel to the z axis. In this axially symmetric case we can also limit ourselves to $m = 0$ and use the expansion (41) in parabolic QS functions. Note that since the potential U is not diagonal in the orbital angular momentum ℓ, one is dealing with scattering of coupled partial waves, and the number of partial waves to be accounted for grows with increasing the quiver amplitude a_0 or the energy E [25]. However, such an energy dependence is absent when using parabolic coordinates, and the size of the matrix representation is only determined by the properties of the potential (60).

We examined the convergence behavior of the scattering amplitude $\tilde{f}^N$, given by formula (49), as the basis size N increases. Specifically, we inspected the ratio of the cross section

$$\frac{\mathrm{d}\sigma^N}{\mathrm{d}\Omega} = |f_C(\theta) + \tilde{f}^N(\theta)|^2 \tag{64}$$

to the Rutherford cross section $\mathrm{d}\sigma_R/\mathrm{d}\Omega = \left|f_C(\theta)\right|^2$. We set the potential parameters $Z = 1$ and $a_0 = 5$. The basis scale parameter is $b = 1$. As shown on the left of Fig. 1 for scattering energy $E = 0.01$ the cross section converges quite rapidly with N in the whole angular interval. The obtained converged ratio agrees very well with the results presented in Fig. 2 of Ref. [25] at small and large scattering angles, but notably disagrees in the intermediate angular region. The agreement at small angles may be attributed to the dominant contribution from the Coulomb amplitude f_C which is exact, and common to both calculations. The authors of Ref. [25] also employed the two-potential formula, but in contrast to our approach they used a partial-wave method for computing the short-range amplitude $\tilde{f}$, which dominates in (47) at large angles. It is well known that the partial-wave expansion better converges at larger rather than smaller angles (see, for instance, Refs. [22,23]). This feature may help in explaining why we observe an agreement between our results and those of Ref. [25] at large angles while a disagreement at intermediate angles; indeed, one could suspect that the number of partial waves taken into account in the calculation of Ref. [25] may suffice for describing scattering at large angles, but may not be enough at intermediate angles. This possible explanation should nevertheless be discarded since the authors of Ref. [25] state that they increased the number of coupled partial waves until the result for the cross section has converged to better than 1%. In order to elucidate this, we further increased N up to 101 in our calculation and found that

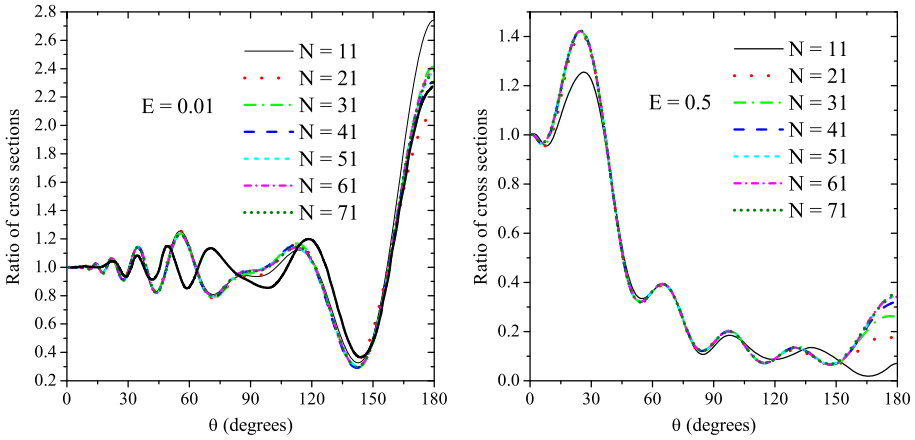

Fig. 1 The ratio of the cross section $d\sigma^N/d\Omega$, calculated for the "dressed" potential (63) with $Z = 1$ and $a_0 = 5$, to the Rutherford cross section $d\sigma_R/d\Omega$. The convergence behavior of the ratio with increasing the basis set size N is shown for $E = 0.01$ (left) and $E = 0.5$ (right). For $E = 0.01$ the result of Ref. [25] is shown with a thick solid line

the curves corresponding to different values of N become almost indistinguishable starting from $N \simeq 60$. Thus, the discrepancy observed at intermediate angles remains unexplained. This said, the discrepancy is not so huge in absolute terms, but is clearly emphasized through the ratio shown in Fig. 2. Finally, in order to show that within our parabolic approach the convergence of the calculations is energy independent, we present on the right of Fig. 1 the numerical results for a higher energy value, $E = 0.5$.

4.3 Scattering by two Coulomb centers

We now focus on the case of an axially symmetric potential that is of importance for applications in molecular physics, in particular for diatomic molecules. Specifically, we consider the electron scattering on the potential generated by a pair of equal point charges $(Z/2)$, separated by a given distance R and located on the z axis at fixed positions $\mathbf{r}_1 = (0, 0, R/2)$ and $\mathbf{r}_2 = (0, 0, -R/2)$. Their Coulomb-like potential reads

$$V(\mathbf{r}) = -\frac{Z/2}{|\mathbf{r} - \mathbf{r}_1|} - \frac{Z/2}{|\mathbf{r} - \mathbf{r}_2|}, \tag{65}$$

and the corresponding "short-range" potential

$$U(\mathbf{r}) = V(\mathbf{r}) + \frac{Z}{r} \tag{66}$$

has singularities (at the point R) on the ξ and η axes. Thus, mathematically this potential does not significantly differ from the potential (60) (except for the type of singularities); the convergence properties should be therefore similar, provided that the truncated matrix representations in the Sturmian basis set (18) of the same size give equally good approximations to the potentials.

We analyzed the convergence behavior of the scattering amplitude in the case of $Z = 2$ simulating, for example, two unscreened protons in a H_2^+ molecular target (a value of $Z = 1$, on the other hand, would take into account a full screening by the bound electron). The ratio of the calculated cross sections $d\sigma^N/d\Omega$ to the Rutherford one is presented in Fig. 2 for the

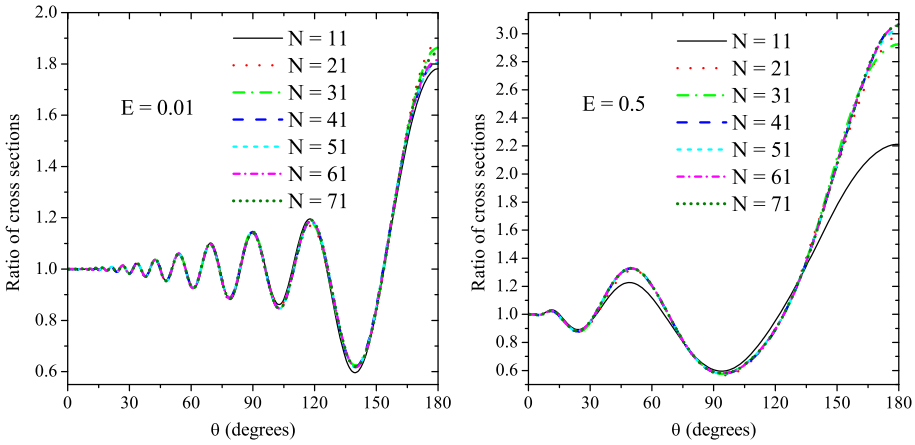

Fig. 2 The ratio of the cross sections $d\sigma^N/d\Omega$ and $d\sigma_R/d\Omega$ for the two-center potential defined by Eq. (65) when $Z = 2$ and the separation distance fixed at $R = 2$. The convergence behavior of the ratio with increasing the basis set size N is shown for $E = 0.01$ (left) and $E = 0.5$ (right)

separation distance $R = 2$ and two energies, $E = 0.01$ and $E = 0.5$. The $R = 2$ value was chosen to mimic the equilibrium distance in the diatomic molecule H_2^+: the calculation, performed with basis scale parameter $b = 3$, shows rapid convergence over the whole angular range. For both energies the rate of convergence is comparable to that observed for the "dressed" Coulomb potential (63).

In both Figs. 1 and 2, convergence in N seems to be slower in the backward direction than in the forward one. There is no physical reason to attribute to this visual feature. It is due to the fact that we are plotting a ratio: the Coulomb contribution is the smallest in the backward direction so that the N dependence appears emphasized in that region.

5 Summary

We have proposed a new approach to quantum scattering theory in parabolic coordinates. The problem is recast as a driven equation with purely incoming or outgoing boundary conditions; the solution in the entire space is approximated by a truncated expansion in terms of parabolic QS functions. The QS asymptotic behavior has been evaluated in closed form, so that the scattering amplitude is expressed directly in terms of the expansion coefficients. The latter are obtained by solving the matrix representation of the driven equation in the complete set of parabolic Sturmians. Evaluation of the matrix includes calculation of the L^2 matrix elements of the Coulomb Green's function for which we derived an analytic form suitable for numerical computations. The short-range part of the interaction is approximated by a truncated matrix in the L^2 basis.

The proposed approach has been implemented and tested by studying electron scattering from three Coulomb-like potentials, two of which possess an axial symmetry. Convergence with increasing basis set size is observed in all cases. For axially symmetric potentials, it is natural to use parabolic rather than spherical coordinates. Indeed, an incident Coulomb wave factorizes in parabolic coordinates, so that the inhomogeneous term of either the Lippmann–Schwinger or driven equations is represented quite compactly for arbitrary energies. On the contrary, the number of terms required in the spherical partial-wave expansion of the

driven term increases as the scattering energy grows. The advantage of using the parabolic coordinates persists also for the case when the direction of the incident particle momentum is different from the symmetry axis. If the z axis is taken to be directed along the symmetry axis, the matrix elements of the operators in (42) are diagonal in m, and hence the equations for each m are solved separately. One can achieve convergence of the quasi-Sturmian expansion separately, for each m-component of the wave function. For the solution it remains then to achieve convergence of the expansion in terms of the angular basis functions.

The parabolic QS approach can be applied to other scattering problems. In particular, one can use it for the treatment of elastic electron scattering on atomic or molecular ions, provided the electron-target interaction is approximated by a local potential that accounts for the exchange and correlation-polarization effects, as done for example in Ref. [26]. Further, the present formalism can be directly extended to multichannel scattering (see, e.g., Ref. [11]), including the case of few-body Coulomb scattering [27]. Specifically, in order to describe a double ionization of atoms by high-energy projectiles, convoluted parabolic QS functions, analogous to those in spherical coordinates [28], can be used as a basis. In the latter case, the z axis is chosen along the incident particle direction.

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Data Availability Statement This manuscript has associated data in a data repository. [Authors' comment: The data of numerical calculations presented in this manuscript are available upon reasonable request by contacting with the corresponding author.].

A The matrix elements of the Green's function

In this appendix we provide the calculation details to perform the four-dimensional integral

$$\mathcal{G}^{|m|(\pm)}_{n_1' n_2';\, n_1 n_2}(\beta, k) = \int_0^\infty \mathrm{d}\xi \int_0^\infty \mathrm{d}\eta \int_0^\infty \mathrm{d}\xi' \int_0^\infty \mathrm{d}\eta' \, \varphi^{|m|}_{n_1'}(\xi)\varphi^{|m|}_{n_2'}(\eta)\, \mathcal{G}^{|m|(\pm)}(k;\xi,\eta;\xi',\eta')\varphi^{|m|}_{n_1}(\xi')\varphi^{|m|}_{n_2}(\eta'). \tag{67}$$

We first make use of the integral representation (17) and interchange integration orders. For the sake of brevity, we consider hereafter only the $(+)$ case. Consider first the integral over ξ'

$$\mathcal{I}_n(\xi) = \int_0^\infty \mathrm{d}\xi' \exp\left\{ i\frac{k}{2}\xi' c - b\xi' \right\} I_\lambda\left(-ik\sqrt{\xi\xi' s}\right)(2b\xi')^{\frac{\lambda}{2}} L_n^\lambda(2b\xi'), \tag{68}$$

where c and s denote $\cosh(z)$ and $\sinh(z)$, respectively. We calculate it using formula (2.19.12, 6) of Ref. [20]

$$\mathcal{I}_n(\xi) = \frac{(-1)^n}{b}\left(ps\sqrt{2x}\right)^\lambda \frac{(1-pc)^n}{(1+pc)^{n+\lambda+1}} \exp\left\{\frac{p^2 s^2 x}{1+pc}\right\} L_n^\lambda\left(-2\frac{p^2 s^2 x}{1-p^2c^2}\right), \tag{69}$$

where $p = -i\frac{k}{2b}$, $x = b\xi$. Then we consider the integral over ξ and perform the following auxiliary integral:

$$\begin{aligned}\mathcal{J}_{mn} &= \int_0^\infty \mathrm{d}\xi\ (2b\xi)^{\frac{\lambda}{2}}\ L_m^\lambda(2b\xi)\mathrm{e}^{-b\xi}\mathcal{I}_n(\xi)\mathrm{e}^{i\frac{k}{2}\xi c} \\ &= (-1)^n\frac{2^\lambda}{b^2}(ps)^\lambda\frac{(1-pc)^n}{(1+pc)^{n+\lambda+1}} \\ &\quad\times\int_0^\infty \mathrm{d}x\, x^\lambda \exp\left\{-x\frac{1+2pc+p^2}{1+pc}\right\} L_m^\lambda(2x)L_n^\lambda\left(-2\frac{p^2s^2x}{1-p^2c^2}\right). \end{aligned} \tag{70}$$

Using formula (2.19.14, 6) of Ref. [20] we obtain

$$\begin{aligned}\mathcal{J}_{mn} &= (-1)^{m+n}\frac{2^\lambda}{b^2}\Gamma(\lambda+1)\,\frac{(\lambda+1)_m(\lambda+1)_n}{m!n!} \\ &\quad\times\frac{(ps)^\lambda(1-p^2)^{m+n}}{(1+2pc+p^2)^{m+n+\lambda+1}}\,{}_2F_1\left(-m,-n;\lambda+1;\frac{4p^2(c^2-1)}{(1-p^2)^2}\right). \end{aligned} \tag{71}$$

The integration over η and η' are performed in exactly the same manner.

Further, for evaluating the Green's function matrix element (67) it remains to integrate over z, and we perform the following integral:

$$\mathcal{K} = -i\mu k\int_0^\infty \mathrm{d}z\ \sinh(z)\left[\coth\left(\frac{z}{2}\right)\right]^{-2i\beta}\mathcal{J}_{n_1',n_1}\,\mathcal{J}_{n_2',n_2}. \tag{72}$$

We use a change of variables

$$x = \left[\tanh\left(\frac{z}{2}\right)\right]^2 \Rightarrow \mathrm{d}x = \sqrt{x}(1-x)\mathrm{d}z \tag{73}$$

to write

$$\mathcal{K} = \frac{i\mu}{2k}\frac{1}{b^2}(1-\zeta^2)^{2\lambda+2}(-\zeta)^{-K}(\lambda!)^2\frac{(\lambda+1)_{n_1'}(\lambda+1)_{n_1}}{n_1'!n_1!}\frac{(\lambda+1)_{n_2'}(\lambda+1)_{n_2}}{n_2'!n_2!}\,\tilde{\mathcal{K}}, \tag{74}$$

where

$$\begin{aligned}\tilde{\mathcal{K}} &= \int_0^1 \mathrm{d}x\, x^{i\beta+\lambda}(1-x)^K(1-\zeta^2x)^{-K-2\lambda-2}\,{}_2F_1\left(-n_1',-n_1;\lambda+1;\left(\frac{1-\zeta^2}{\zeta}\right)^2\frac{x}{(1-x)^2}\right) \\ &\quad\times{}_2F_1\left(-n_2',-n_2;\lambda+1;\left(\frac{1-\zeta^2}{\zeta}\right)^2\frac{x}{(1-x)^2}\right), \end{aligned} \tag{75}$$

and $K = n_1' + n_2' + n_1 + n_2$. The integral $\tilde{\mathcal{K}}$ is calculated as follows. Using the expression of the polynomial

$${}_2F_1\left(-m,-n;\lambda+1;z\right) = \sum_{\ell=0}^{\min(m,n)}\frac{\binom{m}{\ell}\binom{n}{\ell}}{\binom{\lambda+\ell}{\ell}}z^\ell, \tag{76}$$

the product of the two hypergeometric functions becomes the polynomial

$$\sum_{\ell=0}^{u+v} c_\ell \left[\left(\frac{1-\zeta^2}{\zeta} \right)^2 \frac{x}{(1-x)^2} \right]^\ell \tag{77}$$

whose coefficients c_ℓ are

$$c_\ell = \sum_{j=\max(\ell-v,0)}^{\min(\ell,u)} \frac{\binom{n_1}{j}\binom{n_1'}{j}\binom{n_2}{\ell-j}\binom{n_2'}{\ell-j}}{\binom{j+\lambda}{j}\binom{\ell-j+\lambda}{\ell-j}},$$

with $u = \min(n_1, n_1')$ and $v = \min(n_2, n_2')$. We thus have

$$\tilde{\mathcal{K}} = \sum_{\ell=0}^{u+v} c_\ell \left(\frac{1-\zeta^2}{\zeta} \right)^{2\ell} \mathcal{L}_\ell \tag{78}$$

in terms of the integrals

$$\mathcal{L}_\ell = \int_0^1 \mathrm{d}x\, x^{i\beta+\lambda+\ell} (1-x)^{K-2\ell} (1-\zeta^2 x)^{-K-2\lambda-2} \tag{79}$$

which are readily identified as the integral representation of Gauss hypergeometric functions [13] (Eq. (15.3.1))

$$\begin{aligned} \mathcal{L}_\ell &= \frac{\Gamma(i\beta+\lambda+\ell+1)\Gamma(K-2\ell+1)}{\Gamma(i\beta+K+\lambda+2-\ell)} \\ &\quad \times {}_2F_1\left(K+2\lambda+2, \lambda+\ell+1+i\beta; K+\lambda+2-\ell+i\beta; \zeta^2\right) \\ &= \frac{1}{(1-\zeta^2)^{2\lambda+1+2\ell}} \frac{\Gamma(i\beta+\lambda+\ell+1)\Gamma(K-2\ell+1)}{\Gamma(i\beta+K+\lambda+2-\ell)} \\ &\quad \times {}_2F_1\left(K-2\ell+1, -\lambda-\ell+i\beta; K+\lambda+2-\ell+i\beta; \zeta^2\right), \end{aligned} \tag{80}$$

the second equality being obtained through the transformation (15.3.3) of Ref. [13].

Inserting (80) and (78) into (74), and including the basis (19) normalization factors, we find that the matrix element (67) can be expressed as the finite sum (24).

B Asymptotic behavior of the QS functions

In this appendix we explore the large-distance ($r = (\xi+\eta)/2 \to \infty$) behavior of the "radial" part $\mathcal{P}_{n_1 n_2}^{|m|(\pm)}(k;\xi,\eta)$ of the QS functions, starting from the integral representation (30). For the sake of brevity we present here the (+) results only; the (−) case is obtained by complex conjugation. Let us express the Laguerre polynomials L_n^λ in (30) as

$$L_n^\lambda(x) = \sum_{\nu=0}^{n} c_\nu^{(n,\lambda)} x^\nu, \tag{81}$$

where the coefficients $c_\nu^{(n,\lambda)}$ are given by (33) [13]. Thus, the integral in (30) is expressed in terms of the integrals

$$\mathcal{I}_{\mathcal{M},\mathcal{N}} = \int_0^1 \mathrm{d}s (1-s)^{i\beta+\mathcal{M}} (1-\zeta s)^{-i\beta+\mathcal{M}} (1-s-\zeta s)^{\mathcal{N}} \mathrm{e}^{\alpha s}, \tag{82}$$

where

$$\mathcal{M} = \lambda + \nu_1 + \nu_2, \qquad \mathcal{N} = n_1 + n_2 - \nu_1 - \nu_2, \tag{83}$$

and

$$\alpha = 2b(\xi+\eta)\frac{\zeta}{\zeta+1}. \tag{84}$$

Then, using the formal binomial expansions

$$(1-\zeta s)^{-i\beta+\mathcal{M}} = \sum_{\ell=0}^{\infty} \frac{\Gamma(-i\beta+\mathcal{M}+1)}{\Gamma(-i\beta+\mathcal{M}+1-\ell)} \frac{(-\zeta s)^\ell}{\Gamma(\ell+1)} \tag{85}$$

and

$$(1-s-\zeta s)^{\mathcal{N}} = \sum_{\nu=0}^{\mathcal{N}} \binom{\mathcal{N}}{\mathcal{N}-\nu} (1-s)^\nu (-\zeta s)^{\mathcal{N}-\nu}, \tag{86}$$

the integral (82) is given by a sum of integrals

$$\begin{aligned} \mathcal{J}_{\mathcal{M}+\nu,\mathcal{N}+\ell-\nu} &\equiv \int_0^1 \mathrm{d}s (1-s)^{i\beta+\mathcal{M}+\nu} s^{\mathcal{N}+\ell-\nu} \mathrm{e}^{\alpha s} \\ &= \frac{\Gamma(i\beta+\mathcal{M}+\nu+1)\Gamma(\mathcal{N}+\ell-\nu+1)}{\Gamma(i\beta+\mathcal{M}+\mathcal{N}+\ell+2)} \\ &\quad \times M(\mathcal{N}+\ell-\nu+1, i\beta+\mathcal{M}+\mathcal{N}+\ell+2; \alpha) \end{aligned} \tag{87}$$

that are easily identified to be related to the Kummer function M (second equality). Using the asymptotic approximation of the Kummer function for large $|\alpha|$ (see, e.g., Eq. (13.5.1) in Ref. [13]), we find the following (ℓ- and $\mathcal{N}$-independent) asymptotic expression:

$$\mathcal{J}_{\mathcal{M}+\nu,\mathcal{N}+\ell-\nu} \simeq \Gamma(i\beta+\mathcal{M}+\nu+1)\, \alpha^{-(i\beta+\mathcal{M}+\nu+1)}\, \mathrm{e}^{\alpha}. \tag{88}$$

As a consequence, one can retain (for fixed $\mathcal{M}$) only the $\nu = 0$ term in (86), and therefore the integral (82) is approximated by

$$\mathcal{I}_{\mathcal{M},\mathcal{N}} \simeq (-\zeta)^{\mathcal{N}} (1-\zeta)^{-i\beta+\mathcal{M}}\, \Gamma(i\beta+\mathcal{M}+1)\, \alpha^{-(i\beta+\mathcal{M}+1)}\, \mathrm{e}^{\alpha}. \tag{89}$$

Finally, after some algebra and using the fact that $\sqrt{\xi\eta} = \sqrt{x^2+y^2} = r\sin\theta = (1/2)(\xi+\eta)\sin\theta$, we obtain

$$\mathcal{P}_{n_1 n_2}^{\lambda(+)}(k;\xi,\eta) \underset{r\to\infty}{\longrightarrow} \mathcal{A}_{n_1 n_2}^{\lambda(+)}(\theta)\, \frac{\exp\{i\,[kr - \beta\ln(2kr)]\}}{r}, \tag{90}$$

with the amplitudes $\mathcal{A}_{n_1 n_2}^{\lambda(+)}(\theta)$ given by Eq. (32). For the $(-)$ case we simply have $\mathcal{A}_{n_1 n_2}^{\lambda(-)}(\theta) = \left[\mathcal{A}_{n_1 n_2}^{\lambda(+)}(\theta)\right]^*$.

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