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An integral transform of the Coulomb Green's function and off-shell scattering

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Abstract
A closed form expression is derived for the integral $\int_0^\infty \mathrm{d}r'\, \mathrm{e}^{\mathrm{i}qr'} G^{(+)}(r, r')$ and some possible applications of the result are discussed.

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1. Introduction

At a centre of mass energy $E = k^2 + \mathrm{i}\varepsilon$ the s-wave Coulomb Green's function $G^{(+)}(r, r')$ satisfies the differential equation

$$\left[\frac{\mathrm{d}^2}{\mathrm{d}r^2} + k^2 - \frac{2k\eta}{r}\right] G^{(+)}(r, r') = \delta(r - r'), \tag{1}$$

where η is the Sommerfeld parameter. Only the s-wave case is treated here and the subscript $\ell = 0$ is omitted. However, higher partial wave treatment will involve mathematical difficulties. The solution of equation (1) is known in the literature [1] and is given by

$$G^{(+)}(r, r') = 2\mathrm{i}krr'\, \mathrm{e}^{\mathrm{i}k(r+r')}\Gamma(1 + \mathrm{i}\eta)\Phi(1 + \mathrm{i}\eta, 2; -2\mathrm{i}kr_<)\Psi(1 + \mathrm{i}\eta, 2; -2\mathrm{i}kr_>), \tag{2}$$

where $r_<$ and $r_>$ are the larger and smaller values of r and r'. Here Φ and Ψ stand for the regular and irregular confluent hypergeometric functions. Let the function $F(r, r')$ be related to $G^{(+)}(r, r')$ by

$$G^{(+)}(r, r') = r\, \mathrm{e}^{\mathrm{i}kr} F(r, r'). \tag{3}$$

Then the integral transform $\int_0^\infty \mathrm{d}r'\, \mathrm{e}^{\mathrm{i}qr'} F(r, r') = [F(r, r'); q] = \tilde{F}(r, q)$ is related to

$$\tilde{G}^{(+)}(r, q) = \int_0^\infty \mathrm{d}r'\, \mathrm{e}^{\mathrm{i}qr} G^{(+)}(r, r')$$

by

$$\tilde{G}^{(+)}(r, q) = r\, \mathrm{e}^{\mathrm{i}kr}\, \tilde{F}(r, q). \tag{4}$$

In the present paper, a closed form expression for $\tilde{G}^{(+)}(r, q)$ is derived to examine the usefulness of the result in the study of quantum mechanical scattering by the Coulomb field.

Section 2 is devoted to developing a differential equation method for evaluating $\tilde{G}^{(+)}(r, q)$. In section 3 some applications of the expression for $\tilde{G}^{(+)}(r, q)$ are discussed with particular emphasis on off-shell physical and Jost solutions for scattering by the Coulomb potential. Finally, some concluding remarks are presented in section 4.

2. Result for $\tilde{G}^{(+)}(r, q)$

Equation (3) is substituted in equation (1) to get

$$\left[r\frac{\mathrm{d}^2}{\mathrm{d}r^2} + (2 - 2\mathrm{i}k)\frac{\mathrm{d}}{\mathrm{d}r} + (2\mathrm{i}k - 2k\eta)\right] F(r, r') = \mathrm{e}^{-\mathrm{i}kr}\delta(r - r'). \tag{5}$$

Taking the integral transform of the above equation by $\mathrm{e}^{\mathrm{i}qr'}$ with respect to r' and substituting $z = -2\mathrm{i}kr$, equation (5) is obtained as

$$\left[z\frac{\mathrm{d}^2}{\mathrm{d}z^2} + (2 - z)\frac{\mathrm{d}}{\mathrm{d}z} - (1 + \mathrm{i}\eta)\right] \tilde{F}(z, q) = -\left(\frac{1}{2\mathrm{i}k}\right) \mathrm{e}^{\rho z}, \tag{6}$$

with $\rho = \frac{(k-q)}{2k}$.

The two independent solutions of the homogeneous part of equation (6) are given by

$$\Phi(a, c; z) = \left[\frac{\Gamma(c)}{\Gamma(a)}\right] \sum_{n=0}^{\infty} \left[\frac{\Gamma(a+n)}{\Gamma(c+n)}\right] \frac{z^n}{n!} \tag{7}$$

and

$$\bar{\Phi}(a, c; z) = z^{1-c}\Phi(a - c + 1, 2 - c; z) \tag{8a}$$

with

$$a = 1 + \mathrm{i}\eta \qquad \text{and} \qquad c = 2. \tag{8b}$$

Note that for $c = 2$ equation (8a) is not an acceptable solution. However, $\bar{\Phi}(a, c; z)$ tends towards a solution [2] when c approaches 2. In the subsequent discussion that limit is always meant. This is no loss of generalization. See, for example, the treatment of the Coulomb field by Newton [1]. Another solution [2] of equation (6), defined within the same limiting procedure, is

$$\Psi(a, c; z) = \left[\frac{\Gamma(1 - c)}{\Gamma(a - c + 1)}\right] \Phi(a, c; z) + \left[\frac{\Gamma(1 - c)}{\Gamma(a)}\right] \bar{\Phi}(a, c; z). \tag{9}$$

According to Babister [3] the particular solution of the non-homogeneous confluent hypergeometric equation in (6) reads

$$[F(z, q)]_P = -\left(\frac{1}{2\mathrm{i}k}\right) \Lambda_{\rho,1}(1 + \mathrm{i}\eta, 2; z) \tag{10}$$

where

$$\Lambda_{\rho,\sigma}(a, c; z) = \sum_{n=0}^{\infty} \frac{\rho^n}{n!} \theta_{\sigma+n}(a, c; z) \tag{11a}$$

with a, c, ρ, σ constants and

$$\theta_\sigma(a, c; z) = \frac{1}{(c - 1)} \left[\Phi(a, c; z) \int_0^z \mathrm{e}^{-z'} z'^{(\sigma+c-2)} \bar{\Phi}(a, c; z')\, \mathrm{d}z' - \bar{\Phi}(a, c; z) \int_0^z \mathrm{e}^{-z'} z'^{(\sigma+c-2)} \Phi(a, c; z')\, \mathrm{d}z'\right]. \tag{11b}$$

The complete primitive of equation (6) is

$$\tilde{F}(z,q) = A\Phi(1+\mathrm{i}\eta,2;z) + B\bar{\Phi}(1+\mathrm{i}\eta,2;z) - \left(\frac{1}{2\mathrm{i}k}\right)\Lambda_{\rho,1}(1+\mathrm{i}\eta,2;z), \tag{12}$$

where A and B are arbitrary constants. The procedure of determining A and B is as follows. Combine equations (12) and (4) to get

$$\tilde{G}^{(+)}(r,q) = r\,\mathrm{e}^{\mathrm{i}kr}\left[A\Phi(1+\mathrm{i}\eta,2;-2\mathrm{i}kr) + B\bar{\Phi}(1+\mathrm{i}\eta,2;-2\mathrm{i}kr)\right.$$
$$\left. - \left(\frac{1}{2\mathrm{i}k}\right)\Lambda_{\rho,1}(1+\mathrm{i}\eta,2;-2\mathrm{i}kr)\right]. \tag{13}$$

Substitute equation (2) in equation (13) and compare both sides for $r = 0$ to obtain $B = 0$. In view of the above, equation (13) takes the form

$$\tilde{G}^{(+)}(r,q) = r\,\mathrm{e}^{\mathrm{i}kr}\left[A\Phi(1+\mathrm{i}\eta,2;-2\mathrm{i}kr) - \left(\frac{1}{2\mathrm{i}k}\right)\Lambda_{\rho,1}(1+\mathrm{i}\eta,2;-2\mathrm{i}kr)\right]. \tag{14}$$

Taking the limit as $r \to \infty$ is rather tricky. With the help of equations (2), (9) and (11), equation (14) is expressed as

$$2\mathrm{i}k\Gamma(1+\mathrm{i}\eta)r\,\mathrm{e}^{\mathrm{i}kr}\left[\Psi(1+\mathrm{i}\eta,2;-2\mathrm{i}kr)\int_0^r \mathrm{d}r'r'\,\mathrm{e}^{\mathrm{i}(k+q)r'}\Phi(1+\mathrm{i}\eta,2;-2\mathrm{i}kr')\right.$$
$$\left. + \Phi(1+\mathrm{i}\eta,2;-2\mathrm{i}kr)\int_0^r \mathrm{d}r'r'\,\mathrm{e}^{\mathrm{i}(k+q)r'}\Psi(1+\mathrm{i}\eta,2;-2\mathrm{i}kr')\right]$$
$$= r\,\mathrm{e}^{\mathrm{i}kr}\left[A\Phi(1+\mathrm{i}\eta,2;-2\mathrm{i}kr) - \frac{\Gamma(1+\mathrm{i}\eta)}{2\mathrm{i}k}\sum_{n=0}^{\infty}\frac{\rho^n}{n!}\left\{\Phi(1+\mathrm{i}\eta,2;-2\mathrm{i}kr)\right.\right.$$
$$\times \int_0^r \mathrm{d}(-2\mathrm{i}kr')\,\mathrm{e}^{2\mathrm{i}kr'}(-2\mathrm{i}kr')^{n+1}\Psi(1+\mathrm{i}\eta,2;-2\mathrm{i}kr') - \Psi(1+\mathrm{i}\eta,2;-2\mathrm{i}kr)$$
$$\left.\left. \times \int_0^r \mathrm{d}(-2\mathrm{i}kr')\,\mathrm{e}^{2\mathrm{i}kr'}(-2\mathrm{i}kr')^{n+1}\Phi(1+\mathrm{i}\eta,2;-2\mathrm{i}kr')\right\}\right]. \tag{15}$$

Carry out the summation first to get

$$2\mathrm{i}k\Gamma(1+\mathrm{i}\eta)r\,\mathrm{e}^{\mathrm{i}kr}\left[\Psi(1+\mathrm{i}\eta,2;-2\mathrm{i}kr)\int_0^r \mathrm{d}r'r'\,\mathrm{e}^{\mathrm{i}(k+q)r'}\Phi(1+\mathrm{i}\eta,2;-2\mathrm{i}kr')\right.$$
$$\left. + \Phi(1+\mathrm{i}\eta,2;-2\mathrm{i}kr)\int_0^r \mathrm{d}r'r'\,\mathrm{e}^{\mathrm{i}(k+q)r'}\Psi(1+\mathrm{i}\eta,2;-2\mathrm{i}kr')\right]$$
$$= r\,\mathrm{e}^{\mathrm{i}kr}\left[A\Phi(1+\mathrm{i}\eta,2;-2\mathrm{i}kr) - 2\mathrm{i}k\Gamma(1+\mathrm{i}\eta)\left\{\Phi(1+\mathrm{i}\eta,2;-2\mathrm{i}kr)\right.\right.$$
$$\times \int_0^r \mathrm{d}r'r'\,\mathrm{e}^{\mathrm{i}(k+q)r'}\Psi(1+\mathrm{i}\eta,2;-2\mathrm{i}kr') - \Psi(1+\mathrm{i}\eta,2;-2\mathrm{i}kr)$$
$$\left.\left. \times \int_0^r \mathrm{d}r'r'\,\mathrm{e}^{\mathrm{i}(k+q)r'}\Phi(1+\mathrm{i}\eta,2;-2\mathrm{i}kr')\right\}\right]. \tag{16}$$

As $r \to \infty$ the first term on the LHS cancels the last term on the RHS in the above equation to give the desired value of A as

$$A = -\left\{\frac{\mathrm{e}^{\mathrm{i}\pi/2}}{(k+q)(1+\mathrm{i}\eta)}\right\}F\left(1,\mathrm{i}\eta;2+\mathrm{i}\eta;\frac{(q-k)}{(q+k)}\right). \tag{17}$$

In deriving equation (17) the following relations [2, 4] are used,

$$F\left(b,S;1+S+b+d;1-\frac{\mu}{a}\right) = \frac{a^S\Gamma(1+b+S-d)}{\Gamma(1+S-d)\Gamma(S)}\int_0^{\infty}\mathrm{e}^{-ax}x^{S-1}\Psi(b,d;\mu x)\,\mathrm{d}x,$$

with

$$\mathrm{Re}\, S > 0, \qquad 1 + \mathrm{Re}\, S > \mathrm{Re}\, d, \tag{18}$$

and

$$F(a, b; c; z) = (1 - z)^{c-a-b} F(c - a, c - b; c; z). \tag{19}$$

In view of equations (14) and (17) the desired expression for $\tilde{G}^{(+)}(r, q)$ reads

$$\begin{aligned}\tilde{G}^{(+)}(r, q) = r\, \mathrm{e}^{\mathrm{i}kr} \Bigg\{ \left[\frac{\mathrm{e}^{-\mathrm{i}\pi/2}}{(k+q)(1+\mathrm{i}\eta)} \right] F\left(1, \mathrm{i}\eta; 2 + \mathrm{i}\eta; \frac{(q-k)}{(q+k)}\right) \\ \times \Phi(1 + \mathrm{i}\eta, 2; -2\mathrm{i}kr) - \frac{1}{2\mathrm{i}k} \Lambda_{\rho,1}(1 + \mathrm{i}\eta, 2; -2\mathrm{i}kr) \Bigg\}.\end{aligned} \tag{20}$$

When $q \to -q$, equation (20) yields

$$\begin{aligned}\tilde{G}^{(+)}(r, -q) = r\, \mathrm{e}^{\mathrm{i}kr} \Bigg\{ \left[\frac{\mathrm{e}^{-\mathrm{i}\pi/2}}{(k-q)(1+\mathrm{i}\eta)} \right] F\left(1, \mathrm{i}\eta; 2 + \mathrm{i}\eta; \frac{(q+k)}{(q-k)}\right) \\ \times \Phi(1 + \mathrm{i}\eta, 2; -2\mathrm{i}kr) - \frac{1}{2\mathrm{i}k} \Lambda_{1-\rho,1}(1 + \mathrm{i}\eta, 2; -2\mathrm{i}kr) \Bigg\}.\end{aligned} \tag{21}$$

3. Application of the expression for $\tilde{G}^{(+)}(r, q)$

The integral transforms of the outgoing wave Coulomb Green's function can be exploited to construct exact analytical expressions for physical and Jost solutions. The off-shell physical solution $\psi^{(+)}(k, q, r)$ satisfies the inhomogeneous differential equation

$$\left[\frac{\mathrm{d}^2}{\mathrm{d}r^2} + k^2 - \frac{2k\eta}{r} \right] \psi^{(+)}(k, q, r) = (k^2 - q^2) \sin(qr). \tag{22}$$

Fuda and Whiting [5] assumed that the particular integral of equation (22) represents the off-shell physical solution. Thus,

$$\begin{aligned}\psi^{(+)}(k, q, r) &= \frac{(k^2 - q^2)}{2\mathrm{i}} \int_0^\infty \mathrm{d}r' G^{(+)}(r, r')[\mathrm{e}^{\mathrm{i}qr'} - \mathrm{e}^{-\mathrm{i}qr'}] \\ &= \frac{(k^2 - q^2)}{2\mathrm{i}} [\tilde{G}^{(+)}(r, q) - \tilde{G}^{(+)}(r, -q)].\end{aligned} \tag{23}$$

In view of equations (20) and (21), equation (23) yields

$$\begin{aligned}\psi^{(+)}(k, q, r) = -\frac{1}{2(1+\mathrm{i}\eta)} r\, \mathrm{e}^{\mathrm{i}kr} \Phi(1 + \mathrm{i}\eta, 2; -2\mathrm{i}kr) \left[(k-q) F\left(1, \mathrm{i}\eta; 2 + \mathrm{i}\eta; \frac{(q-k)}{(q+k)}\right) \right. \\ \left. - (k+q) F\left(1, \mathrm{i}\eta; 2 + \mathrm{i}\eta; \frac{(q+k)}{(q-k)}\right) \right] \\ - \mathrm{Im} \left[\frac{(k^2 - q^2)}{2\mathrm{i}k} r\, \mathrm{e}^{\mathrm{i}kr} \Lambda_{\rho,1}(1 + \mathrm{i}\eta, 2; -2\mathrm{i}kr) \right].\end{aligned} \tag{24}$$

Following Babister's relation [3]

$$\Lambda_{1-\rho,\sigma}(a, c; z) = \mathrm{e}^{(z - \mathrm{i}\pi\sigma)} \Lambda_{\rho,\sigma}(c - a, c; z\, \mathrm{e}^{\mathrm{i}\pi}), \tag{25}$$

one can easily prove that the quantity $\frac{(k^2-q^2)}{2\mathrm{i}k} r\, \mathrm{e}^{\mathrm{i}kr} \Lambda_{\rho,1}(1 + \mathrm{i}\eta, 2; -2\mathrm{i}kr)$ is real. After certain algebraic manipulation, with the help of the relations [1, 2]

$$\begin{aligned}F(a, b; c; z) = \frac{\Gamma(c)\Gamma(b-a)}{\Gamma(b)\Gamma(c-a)} (-z)^{-a} F(a, 1 - c + a; 1 - b + a; z^{-1}) \\ + \frac{\Gamma(c)\Gamma(a-b)}{\Gamma(a)\Gamma(c-b)} (-z)^{-b} F(b, 1 - c + b; 1 - a + b; z^{-1}),\end{aligned} \tag{26}$$

$$T(k,q,k^2) = \frac{1}{\mathrm{i}\pi q f(k)}\,[f(k,q) - f(k-q)]\,, \tag{27}$$

and

$$\varphi(k,r) = \frac{\mathrm{e}^{\pi\eta/2}}{2k}\left[\frac{\mathrm{e}^{-\mathrm{i}\pi/2}}{\Gamma(1-\mathrm{i}\eta)}f(k,r) + \frac{\mathrm{e}^{\mathrm{i}\pi/2}}{\Gamma(1+\mathrm{i}\eta)}f(-k,r)\right], \tag{28}$$

the regular solution, equation (24), is obtained as

$$\begin{aligned}\psi^{(+)}(k,q,r) = -\frac{1}{2}\pi q T(k,q,k^2) f(k,r) + \mathrm{Im}\Bigg[&\frac{\mathrm{e}^{\mathrm{i}\pi/2}(q-k)}{(1+\mathrm{i}\eta)}F\left(1,\mathrm{i}\eta;2+\mathrm{i}\eta;\frac{(q-k)}{(q+k)}\right)\\ &\times r\,\mathrm{e}^{\mathrm{i}kr}\Phi(1+\mathrm{i}\eta,2;-2\mathrm{i}kr) - 2\mathrm{i}k\Gamma(1+\mathrm{i}\eta)\left(\frac{(q+k)}{(q-k)}\right)^{\mathrm{i}\eta}\\ &\times r\,\mathrm{e}^{\mathrm{i}kr}\Psi(1+\mathrm{i}\eta,2;-2\mathrm{i}kr) - \frac{(k^2-q^2)}{2\mathrm{i}k}r\,\mathrm{e}^{\mathrm{i}kr}\Lambda_{\rho,1}(1+\mathrm{i}\eta,2;-2\mathrm{i}kr)\Bigg].\end{aligned} \tag{29}$$

The off-shell physical solution is related to half-shell T-matrix and off-shell Jost solution by

$$\psi^{(+)}(k,q,r) = -\tfrac{1}{2}\pi q T(k,q,k^2) f(k,r) + \mathrm{Im}\, f(k,q,r). \tag{30}$$

On comparing equations (29) and (30) the off-shell Jost solution reads

$$\begin{aligned}f(k,q,r) = r\,\mathrm{e}^{\mathrm{i}kr}\Bigg[&\frac{\mathrm{e}^{\mathrm{i}\pi/2}(q-k)}{(1+\mathrm{i}\eta)}F\left(1,\mathrm{i}\eta;2+\mathrm{i}\eta;\frac{(q-k)}{(q+k)}\right)\Phi(1+\mathrm{i}\eta,2;-2\mathrm{i}kr)\\ &- 2\mathrm{i}k\Gamma(1+\mathrm{i}\eta)\left(\frac{(q+k)}{(q-k)}\right)^{\mathrm{i}\eta}\Psi(1+\mathrm{i}\eta,2;-2\mathrm{i}kr)\\ &- \frac{(k^2-q^2)}{2\mathrm{i}k}\Lambda_{\rho,1}(1+\mathrm{i}\eta,2;-2\mathrm{i}kr)\Bigg],\end{aligned} \tag{31}$$

which is consistent with the earlier result [6] obtained by a different method.

Some years ago we [7] have also derived an expression for the s-wave Coulomb off-shell Jost solution from its integral representation in terms of products of confluent hypergeometric functions. But the expression in equation (31) or in [6] is much more simpler than the previous one. A couple of useful checks are made on the expression for the Coulomb off-shell Jost solution with particular emphasis on their limiting behaviour and on-shell discontinuity [8]. For example, in the limit of no Coulomb field, $f(k,q,r) = \mathrm{e}^{\mathrm{i}kr}$. Secondly,

$$f(k,q) = Lt_{r\to 0} f(k,q,r) = \left(\frac{(q+k)}{(q-k)}\right)^{\mathrm{i}\eta} \tag{32}$$

and

$$f(k,q) = Lt_{q\to k}\left\{\frac{\mathrm{e}^{\pi\eta/2}}{\Gamma(1+\mathrm{i}\eta)}\left(\frac{(q+k)}{(q-k)}\right)^{\mathrm{i}\eta} f(k,q,r)\right\}. \tag{33}$$

Equations (32) and (33) can easily be verified from the results in equation (31), which are in agreement with earlier results [1, 9].

4. Concluding remarks

A closed form expression for the integral $\int_0^\infty \mathrm{d}r'\,\mathrm{e}^{\mathrm{i}qr'}G^{(+)}(r,r')$ for motion in the Coulomb field is derived and some of its applications, particularly the off-shell Jost solution, are discussed. By exploiting the relation that exists between fully off-shell T-matrix and $\psi^{(+)}(k,q,r)$, one will be in a position to write an uncomplicated expression for the off-shell T-matrix. The matter will be reported in detail in a subsequent paper. This conjecture represents a straightforward approach to deal with off-shell scattering on the Coulomb potential. Also the closed form expression for $f(k,q,r)$ is believed to be useful for the description of the physical processes in atomic and molecular physics [10].

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