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Off-shell Jost solution for scattering by a Coulomb field

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A relatively uncomplicated mathematical prescription based on the theory of ordinary differential equations together with certain properties of higher transcendental functions is used to obtain a useful analytical expression for the *s*-wave Coulomb off-shell Jost solution.

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Based on a coordinate-space approach [1] to the T matrix, Fuda and Whiting [2] have introduced an off-energy-shell generalization of the Jost function. [3] At an energy $E=k^2>0$ the Jost function $f_\ell(k)$ is determined by the behavior of the irregular solution $f_\ell(k,r)$ of the radial Schrödinger equation near the origin. The off-shell Jost function $f_\ell(k,q)$ is also determined from irregular solution of an inhomogeneous Schrödinger equation in the same way as $f_\ell(k)$ is obtained from $f_\ell(k,r)$. Some years ago we [4] derived an expression for the s-wave Coulomb off-shell Jost solution in terms of products of confluent hypergeometric functions. This has been achieved from an integral representation for $f_\ell(k,q,r)$.

In this paper we shall present a relatively uncomplicated mathematical prescription based on the theory of ordinary differential equations together with certain properties of higher transcendental functions to derive an expression for the s-wave off-shell Jost solution for scattering by Coulomb field. Here we omit the subscript $\ell=0$. The treatment of higher partial wave will involve mathematical complication.

The off-shell Jost solution $f(k,q,r)$ for a spherically symmetric potential V(r) satisfies the Schrödinger-like equation

$$[d^2/\mathrm{d}r^2+k^2-V(r)]f(k,q,r)=(k^2-q^2)e^{iqr}. \tag{1}$$

The function $f(k,q,r)$ has asymptotic normalization

$$f(k,q,r)_{r\to\infty}\sim e^{iqr}. \tag{2}$$

When $q=\pm k$, $f(k,q,r)$ goes over into the two irregular solutions of the Schrödinger equation which enter into the theory of ordinary Jost function $f(k)$ and we have

$$f(\pm k,r)=f(k,\pm k,r). \tag{3}$$

Equations (2) and (3) hold when the first and second moments of $V(r)$ are finite. The Coulomb case needs separate considerations.

With $V(r)=2k\eta/r$ and changing the dependent and independent variables in Eq. (1) by substituting

$$f(k,q,r)=\mathrm{r}e^{iqr}g(k,q,r), \tag{4a}$$

$$z=-2ikr, \tag{4b}$$

we have

$$[zd^2/dz^2+(c-z)d/dz-a]g(k,q,z)=-[(k^2-q^2)/2ik]e^{\rho z}, \tag{5}$$

where a, c, and ρ are constants with values $a=1+i\eta$, $c=2$, and $\rho=(k-q)/2k$.

The complementary functions of Eq. (5) are given by confluent hypergeometric functions

$$\Phi(a,c;z)=\Gamma(c)/\Gamma(a)\sum_{n=0}^{\infty}[\Gamma(a+n)z^n]/[\Gamma(c+n)\Gamma(n+1)] \tag{6}$$

and

$$\overline{\Phi}(a,c;z)=z^{1-c}\Phi(a-c+1,2-c;z). \tag{7}$$

Note that, for $c=2$, $\overline{\Phi}$ is not an acceptable solution of Eq. (1). However, $\overline{\Phi}$ tends towards the solution [5] of Eq. (1) when c approaches 2. In our subsequent discussions we shall always mean that limit. This is no loss of generalization. See, for example, the treatment of Coulomb field by Newton. [6] Another solution of Eq. (1) defined within the framework of the same limiting procedure is

$$\Psi(a,c;z)=[\Gamma(1-c)/\Gamma(a-c+1)]\Phi(a,c;z)+[\Gamma(c-1)/\Gamma(a)]\overline{\Phi}(a,c;z). \tag{8}$$

Babister [7] notes that the particular solution of the inhomogeneous confluent hypergeometric equation

$$[zd^2/dz^2+(c-z)d/dz-a]y=z^{\sigma-1} \tag{9}$$

reads as

$$\theta_\sigma(a,c;z)=z^\sigma\sum_{n=0}^{\infty}[\Gamma(\sigma+a+n)\Gamma(\sigma)\Gamma(\sigma+c-1)]z^n/[\Gamma(\sigma+a)\times\Gamma(\sigma+n+1)\Gamma(\sigma+c+n)]$$
$$=[z^\sigma/\sigma(\sigma+c-1)]{}_2F_2(1,\sigma+a;\sigma+1,\sigma+c;z). \tag{10}$$

Thus the particular solution of Eq. (5) is obtained as

$$g_p(k,q,z) = -[(k^2-q^2)/2ik]\sum_{n=0}^{\infty}[\rho^n/n!]\theta_{n+1}(1+i\eta,2;z). \tag{11}$$

Combining Eqs. (6), (8), and (11) the general solution of Eq. (5) is written as

$$g(k,q,z) = A\Phi(1+i\eta,2;z) + B\Psi(1+i\eta,2;z) - [(k^2-q^2)/2ik]\sum_{n=0}^{\infty}[\rho^n/n!]\theta_{n+1}(1+i\eta,2;z). \tag{12}$$

Therefore the Jost solution is obtained as

$$f(k,q,r) = A\, re^{ikr}\Phi(1+i\eta,2;-2ikr) + B\, re^{ikr}\Psi(1+i\eta,2;-2ikr) - re^{ikr}[(k^2-q^2)/2ik] \times\sum_{n=0}^{\infty}[\rho^n/n!]\theta_{n+1}(1+i\eta,2;-2ikr), \tag{13}$$

with A and B are two arbitrary constants.

The on- and off-shell Jost functions $f_\ell(k)$ and $f_\ell(k,q)$ are defined by [6]

$$f_\ell(k) = \lim_{r\to 0} f_\ell(k,r)(-2ikr)^\ell \ell!/(2\ell)! \tag{14}$$

and

$$f_\ell(k,q) = \lim_{r\to 0} f_\ell(k,q,r)(-2iqr)^\ell \ell!/(2\ell)!\,. \tag{15}$$

The off-shell Coulomb Jost function [8] for $\ell=0$ is extremely simple and is written as

$$f(k,q) = [(q+k)/(q-k)]^{i\eta}. \tag{16}$$

Thus the two constants A and B in Eq. (13) can be determined by exploiting the values of $f(k,q,r)$ at $r=0$ and ∞. Using the boundary condition at $r=0$ in Eq. (13), we have

$$B = -2ik\Gamma(1+i\eta)[(q+k)/(q-k)]^{i\eta}. \tag{17}$$

In the above we have used the fact that $\lim_{z\to 0}\Psi(a,c;z) \sim z^{1-c}[\Gamma(c-1)/\Gamma(a)]$ together with Eqs. (15) and (16). From Eqs. (13) and (17) we obtain

$$f(k,q,r) = A\, re^{ikr}\Phi(1+i\eta,2;-2ikr) - 2ik\Gamma(1+i\eta)[(q+k)/(q-k)]^{i\eta}re^{ikr} \times\Psi(1+i\eta,2;2ikr) - re^{ikr}[(k^2-q^2)/2ik] \times\sum_{n=0}^{\infty}[\rho^n/n!]\theta_{n+1}(1+i\eta,2;-2ikr). \tag{18}$$

Evaluation of constant A from the boundary condition as $r\to\infty$ is rather tricky. To that end Eq. (18) is rewritten in the form

$$f(k,q,r) = A\, re^{ikr}\Phi(1+i\eta,2;-2ikr) - 2ikr\Gamma(1+i\eta) \times[(q+k)/(q-k)]^{i\eta}re^{ikr}\Psi(1+i\eta,2;2ikr) + (k^2-q^2)\int_0^r G^R(r,r')e^{iqr'}dr'. \tag{19}$$

The following facts are used in writing Eq. (19) from Eq. (18). Here $\theta_\sigma(a,c;z)$ is expressed in terms of indefinite integrals [7,8] involving $\Phi(\bullet)$ and $\overline{\Phi}(\bullet)$ as

$$\theta_\sigma(a,c;z) = 1/(c-1)[\Phi(a,c;z)\int_0^z ds\, s^{\sigma+c-2}e^{-s}\overline{\Phi}(a,c;s) - \overline{\Phi}(a,c;z)\int_0^z ds\, s^{\sigma+c-2}e^{-s}\Phi(a,c;s)] \tag{20}$$

and the well-known Coulomb regular Green function

$$G^R(r,r') = [\varphi(k,r)f(k,r') - \varphi(k,r')f(k,r)]/f(k), = 2ikrr'e^{ik(r+r')}[\overline{\Phi}(1+i\eta,2;-2ikr) \times\Phi(1+i\eta,2;-2ikr') - \overline{\Phi}(1+i\eta,2;-2ikr') \times\Phi(1+i\eta,2;-2ikr)] \tag{21}$$

for $r'<r$ and zero elsewhere, with $\varphi(k,r)$ and $f(k,r)$, the regular and irregular Coulomb solutions respectively. As $r\to\infty$, Eq. (19) together with the transposed operator relation $\int\varphi(O\Psi)=\int\Psi(\tilde{O}\varphi)$, where $\tilde{O}=O$ and the differential equations for $G^R(r,r'),\varphi(k,r)$ and $f(k,r)$ yield

$$A = [i(q-k)/(1+i\eta)]F(1,i\eta;2+i\eta;(q-k)/(q+k)). \tag{22}$$

From Eqs. (13), (17), and (22) the desired expression for $f(k,q,r)$ is obtained as

$$f(k,q,r) = 2ik\Gamma(1+i\eta)re^{ikr}\{[(q-k)/\{2k\Gamma(2+i\eta)\}] \times F(1,i\eta;2+i\eta;(q-k)/(q+k))\Phi(1+i\eta,2;-2ikr) - [(q+k)/(q-k)]^{i\eta}\Psi(1+i\eta,2;-2ikr)\} - re^{ikr}[(k^2-q^2)/2ik]\sum_{n=0}^{\infty}[\rho^n/n!]\theta_{n+1}(1+i\eta,2;-2ikr). \tag{23}$$

Using the integral representations [5,7] of $\Phi(\bullet)$ and $\Psi(\bullet)$ and the value of $\theta_\sigma(1,2;z)$, we have checked that when $\eta=0$, $f(k,q,r)=e^{iqr}$. Other useful checks on Eq. (23) consist in showing that

$$f(k,q,0) = f(k,q) = [(q+k)/(q-k)]^{i\eta}, \tag{24}$$

$$f(k,r) = \lim_{q\to k}[(q-k)/(q+k)]^{i\eta}[e^{\pi\eta/2}/\Gamma(1+i\eta)]f(k,q,r), \tag{25}$$

$$f(k,q,r)_{r\to\infty} \sim e^{iqr}. \tag{26}$$

The above facts hold when an arbitrary short-range potential is also added to the Coulomb potential. Therefore, it seems to be very interesting to have explicit expressions for off-shell Jost solution and T matrix for motion in the Coulomb plus a rather general short-range interaction. This will be reported in detail in a subsequent paper.

By using a Sturmian discretization of Coulomb Green's function, Dube and Broad [9] have constructed some useful algorithms to compute the values of the outgoing-wave off-shell Coulomb function $\psi^{(+)}(k,q,r)$. But our result for $f(k,q,r)$ and $f(k,q)$ (Ref. [8]) can be used to construct an exact analytical expression for $\psi^{(+)}(k,q,r)$. Making use of

$$\psi^{(+)}(k,q,r) = [1/2i][\{[f(k,q) - f(k,-q)]/f(k)\}f(k,r) + \{f(k,q,r) - f(k,-q,r)\}], \tag{27}$$

we have obtained

$$\begin{aligned}\psi^{(+)}(k,q,r) = {} & [1/2ik]re^{ikr}\Phi(1+i\eta,2;-2ikr)[(q-k) \\ & \times F(1,i\eta;2+i\eta;(q-k)/(q+k)) + (k+q) \\ & \times F(1,i\eta;2+i\eta;(q+k)/(q-k)] \\ & - \mathrm{Im}\{[(k^2-q^2)/2ik]r\, e^{ikr}\Lambda_{\rho,1}(1+i\eta,2;-2ikr)\},\end{aligned} \tag{28}$$

where

$$\begin{aligned}\Lambda_{\rho,\sigma}(a,c,z) = {} & z^{\sigma}\sum_{n=0}^{\infty}[\Gamma(\sigma+a+n)\Gamma(\sigma)\Gamma(\sigma+c-1)]/\Gamma(\sigma+a) \\ & \times\Gamma(\sigma+n+1)\Gamma(\sigma+c+n)F_{(n+1)} \\ & \times(\sigma,\sigma+c-1;\sigma+a;\rho)z^n \\ = {} & \sum_{n=0}^{\infty}[\rho^n/n\,!\,]\theta_{\sigma+n}(a,c,z).\end{aligned} \tag{29}$$

Here $F_{(n+1)}$ stands for the first $(n+1)$ terms of the hypergeometric series [5,7] with the given parameters.

Given the expression for $\psi^{(+)}(k,q,r)$, one will be in a position to write an uncomplicated expression for the off-shell Coulomb T matrix which is expected to circumvent in a rather natural way the typical difficulties associated with the derivation [10] of T(•) from the known expression for the three-dimensional Coulomb T matrix.[11]

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