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Integral representations of the Jost function

B. Talukdar, U. Laha,* and U. Das†
Department of Physics, Visva-Bharati, Santiniketan 731 235, India
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Apparently different criteria are used to arrive at the integral representations of Jost functions. In dealing with this we present a guideline to rederive these results only from the Volterra integral equation satisfied by the Jost solutions. Both on- and off-shell Jost-type functions are considered. Using one of our formal results, we derive a useful expression for the *s*-wave Coulomb off-shell Jost solution.

At an energy $E=k^2>0$ the Jost function[1] $f_l(k)$ is determined by the behavior of the irregular solution $f_l(k,r)$ of the radial Schrödinger equation near the origin. This function has played a central role in examining the analytic properties of partial-wave scattering amplitudes. For a given angular momentum l, there exist two integral representations[2] for $f_l(k)$; one in terms of the irregular solution $f_l(k,r)$ and the other in terms of the regular solution $\varphi_l(k,r)$. The integral representation involving the irregular solution follows in a rather straightforward way from the integral equation for $f_l(k,r)$. In contrast to this the other integral representation is derived with particular attention to the asymptotic behavior of $\varphi_l(k,r)$.

In the recent past, Fuda and Whiting[3] have introduced an off-energy-shell generalization of the Jost function. The off-shell Jost function $f_l(k,q)$ is also determined from the irregular solution of an inhomogeneous Schrödinger equation in the same way as $f_l(k)$ is obtained from $f_l(k,r)$. Here q is an off-shell momentum. The function $f_l(k,q)$ is normalized so that, for scattering on short-range potentials, $f_l(k,q)$ becomes the ordinary Jost function $f_l(k)$ on the energy shell, i.e., when $q=k$. For the Coulomb potential, however, $f_l(k,q)$ exhibits a discontinuity[4] as $q\to k$. The half-off-shell T matrix can be expressed directly in terms of off-shell Jost functions. Also by exploiting the relations which exist between the fully off-shell T matrix elements and half-off-shell T matrices, one can write the off-shell T matrix in terms of the off-shell Jost function. As with $f_l(k)$, the function $f_l(k,q)$ has also two integral representations. One of these is given in terms of $f_l(k,q,r)$, the off-shell Jost solution. This result follows from the integral equation for $f_l(k,q,r)$. The other one involves a free-particle off-shell solution and the on-shell function $\varphi_l(k,r)$. The derivation of the second integral representation is rather tricky. For example, Fuda[5] obtained it by using a momentum space formulation of the off-shell Jost function and taking recourse to Kowalski's generalization of the Sasakawa method.[6] Thus it is clear that we do not have a common basis to derive these integral representations.

One of our objectives in this work is to look for a unified prescription to arrive at these integral representations. We shall achieve this by writing a representation for $f_l(k,q,r)$, which has not hitherto been discussed in the literature. Further, we shall demonstrate that this new representation provides a natural basis for expressing the off-shell Coulomb Jost solution in simple analytical form. The result for the Coulomb off-shell Jost function has appeared in a number of publications,[7] while the result for the Coulomb off-shell Jost solution is new to our knowledge. For clarity of presentation we shall deal only with the *s*-wave case and omit the subscript, $l=0$. The treatment of the higher partial wave will not involve any new mathematical complication.

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

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

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

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

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 the 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. We shall introduce them while dealing with the Coulomb problem.

With Fuda and Whiting[3] we assume that the particular integral of Eq. (1) represents the off-shell Jost solution. We thus write

$$f(k,q,r)=(k^2-q^2)\int_r^\infty G^I(k,r,r')e^{iqr'}dr' , \tag{4}$$

where $G^I(k,r,r')$ stands for the irregular Green's function for motion in the potential $V(r)$ and is given by

$$G^I(k,r,r')=\begin{cases}0, & r'<r\\ [\phi(k,r')f(k,r) \\ \quad -\phi(k,r)f(k,r')]/f(k), & r'>r .\end{cases} \tag{5}$$

Here $\phi(k,r)$ and $f(k,r)$ are the regular and irregular solution of the Schrödinger equation for $V(r)$. Obviously, $f(k)$ is the corresponding Jost function. From Eqs. (4) and (5) and the radial Schrödinger equation, we have found that

$$f(k,q,r)=e^{iqr}+\frac{1}{f(k)}\int_r^\infty[f(k,r)\phi(k,r')-\phi(k,r)f(k,r')]\times V(r')e^{iqr'}dr' . \tag{6}$$

In deriving Eq. (6) we have used the boundary conditions[2] on $f(k,r)$ and $\phi(k,r)$. Interestingly, Eq. (6) is the formal solution of the integral equation

$$f(k,q,r)=e^{iqr}+\int_r^\infty G_0^I(k,r,r')V(r')f(k,q,r')dr' \tag{7}$$

with $G_0^I(k,r,r')$, the free-particle irregular Green's function written as

$$G_0^I(k,r,r')=\begin{cases}0, & r'<r\\ -k^{-1}\sin k(r-r'), & r'>r .\end{cases} \tag{8}$$

Although Eq. (6) appears to follow in a rather straightforward way from Eq. (8), it was never used to derive the integral representations for Jost functions. In the on-shell limit Eq. (6) gives

$$f(k,r)=e^{ikr}+\frac{1}{f(k)}\int_r^\infty[f(k,r)\phi(k,r')-\phi(k,r)f(k,r')]\times V(r')e^{ikr'}dr' . \tag{9}$$

From Eqs. (6) and (9) the integral representations of $f(k,q)$ and $f(k)$ are obtained as

$$f(k,q)=f(k,q,0)=1+\int_0^\infty e^{iqr}V(r)\phi(k,r)dr \tag{10}$$

and

$$f(k)=f(k,0)=1+\int_0^\infty e^{ikr}V(r)\phi(k,r)dr . \tag{11}$$

Thus in contrast to the derivation of Fuda[5] and of Newton[2] we have arrived at Eqs. (10) and (11) only by using the formal solution of the familiar integral equations for $f(k,q,r)$ and $f(k,r)$. Note that the other integral representations follow directly from Eq. (7) and its on-shell version. This indicates that the integral equation for the Jost solution and its formal solution provide a common basis for deriving all the integral representations.

An important virtue of Eq. (10) is that it is applicable both for short-range and Coulomb potentials. We, therefore, venture to suggest that Eq. (6) will also hold good for the Coulomb potential $V^C(r)=2\eta k/r$ with η, the Sommerfeld parameter. Using the regular and irregular solutions[2] of the Coulomb potential as well as the Coulomb Jost function in Eq. (6) we can write the Coulomb off-shell Jost solution in the form

$$f^C(k,q,r)=e^{iqr}-\Gamma(1+i\eta)re^{ikr}[2ik\Psi(1+i\eta,2;-2ikr)I_1(r)+e^{-\pi\eta/2}\Phi(1+i\eta,2;-2ikr)I_2(r)] , \tag{12}$$

where Φ ( ) and Ψ ( ) stand for the regular and irregular confluent hypergeometric functions and the superscript C refers to the Coulomb potential. The quantities $I_1(r)$ and $I_2(r)$ are given by

$$I_1(r)=2\eta k\int_r^\infty e^{i(k+q)r'}\Phi(1+i\eta,2;-2ikr')dr' \tag{13a}$$

and

$$I_2(r)=-4i\eta k^2e^{\pi\eta/2}\int_r^\infty e^{i(k+q)r'}\Psi(1+i\eta,2;-2ikr')dr' . \tag{13b}$$

We have evaluated the values of $I_1(r)$ and $I_2(r)$ by using the integral representations[8] of the Φ ( ) and Ψ ( ) functions and arrived at

$$f^C(k,q,r)=e^{iqr}\left\{1+\frac{4\eta k^2r\Gamma(1+i\eta)}{k+q}\left[\left[\frac{1}{\Gamma 1-i\eta)}\Psi(1+i\eta,2;-2ikr)+e^{-\pi\eta}\Phi(1+i\eta,2;-2ikr)\right]S(r)+\frac{k+q}{|\Gamma(1+i\eta)|^2}\Psi(1+i\eta,2;-2ikr)T(r)\right]\right\} , \tag{14}$$

where $S(r)$ and $T(r)$ are given by

$$S(r)=\sum_{n=0}^{\infty}\frac{(2ikr)^n}{[\Gamma(1+i\eta)]^2}\Gamma(n-i\eta)\,{}_2F_1\left[1,1+i\eta;1+i\eta-n;\frac{q-k}{q+k}\right] \tag{15a}$$

and

$$T(r)=\frac{1}{2k}\left[\frac{q+k}{q-k}\right]^{i\eta}\sum_{n=0}^{\infty}\frac{\Gamma(1+n-i\eta)\Gamma(i\eta-n)}{\Gamma(n+1)}\left[\frac{q-k}{2k}\right]^n(2ikr)^n . \tag{15b}$$

The series in Eqs. (15a) and (15b) are uniformly convergent and can therefore be evaluated on a digital computer. Making use of the fact that $\Psi(a,c;z)\sim_{z\to 0}z^{1-c}\Gamma(c-1)/\Gamma(a)$ and $\Phi(a,c;z)\sim_{z\to 0}1$ and also that only $n=0$ terms of $S(r)$

and $T(r)$ remain nonvanishing near the origin, we can obtain the Jost function $f^C(k,q)$ from Eq. (14). We have[4]

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

Another useful check on Eq. (14) consists in showing that[4]

$$f^C(k,r)=\lim_{q\to k}\left[\frac{q-k}{q+k}\right]^{i\eta}\frac{e^{\pi\eta/2}}{\Gamma(1+i\eta)}f^C(k,q,r) . \tag{17}$$

Equation (17) can easily be verified from our results in Eqs. (14)and (15). As in the case of short-range potentials $f^C(k,q,r)$ also goes like e^{iqr} as $r\to\infty$. This is not apparent from Eq. (14). However, one can write Eq. (14) in the equivalent form

$$f^C(k,q,r)=e^{iqr}\left[1+\frac{4\eta k^2 r}{k+q}\sum_{n=0}^{\infty}\left[\frac{2k}{k+q}\right]^n\frac{\Gamma(1+i\eta+n)}{\Gamma(n+2)}\times\{\Psi(1+i\eta,2;-2ikr)\Phi(1-i\eta,n+2;2ikr)-\Phi(1-i\eta,2;2ikr)(-1)^n\Gamma(n+2)\Psi(1+n+i\eta,n+2;-2ikr)\}\right] . \tag{18}$$

Using the asymptotic values[8] of Φ ( ) and Ψ ( ) in Eq. (18), one can check that $f^C(k,q,r)\sim_{r\to\infty}e^{iqr}$.

By using a Sturmian discretization of the Coulomb Green's function Dube and Broad[9] have recently constructed some useful algorithms to compute the values of the outgoing-wave off-shell Coulomb function $\Psi_l^{C(+)}(k,q,r)$. But our results for $f^C(k,r)$ and $f^C(k,q,r)$, and their subsequent higher partial-wave generalization can be used to construct an exact analytic expression for $\Psi_l^{C(+)}(k,q,r)$. Given the expression for $\Psi_l^{C(+)}(k,q,r)$ one will be in a position to write a uncomplicated expression for the partially projected off-shell Coulomb T matrix in terms of the formula

$$T_l^C(p,q,k^2)=\frac{2}{\pi pq}\int_0^{\infty}dr\,\hat{j}_l(pr)V^C(r)\Psi_l^{C(+)}(k,q,r) \tag{19}$$

with $\hat{j}_l(x)$ the Riccati Bessel function. This conjecture represents a straightforward approach to deal with off-energy-shell scattering on the Coulomb potential. It is expected to circumvent in a rather natural way the typical difficulties associated with derivation[10] of T_l^C( ) from the known expression for the three-dimensional Coulomb T matrix.[11]

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*Permanent address: Physics Department, Regional Institute of Technology, Jamshedpur, Bihar, India.

†Permanent address: Department of Physics, Abhedananda Mahavidyalaya, Sainthia 731 234, India.

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