NASA TECHNICAL NOTE

NASA TN D-2781

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NASA TN D-2781

EFFECTS OF SHIELDING ON THE COULOMB T MATRIX

by William F. Ford

Lewis Research Center

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NATIONAL AERONAUTICS AND SPACE ADMINISTRATION • WASHINGTON, D. C. • APRIL 1965

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SUMMARY

The Coulomb T matrix is defined as the limiting value of the T matrix for a screened Coulomb potential when the screening is slowly turned off. Study of this limiting process is facilitated by an expansion in spherical harmonics, and the $\ell = 0$ term is treated in detail. The amplitude of the T matrix changes rapidly as a function of energy in the vicinity of certain critical points. The precise value of the T matrix in these regions requires that screening be taken into account, and the appropriate formulas are derived. An expression for the T matrix previously derived by Hostler is shown to be correct except in the critical regions.

INTRODUCTION

A quantity of considerable interest in the formal theory of scattering is the operator T, defined symbolically by

$$T = V + V \frac{1}{E + i\epsilon - K - V} V \tag{1}$$

Here K is the Hamiltonian for the system in the absence of interaction, and V is the interaction giving rise to the scattering. The total energy of the system is denoted by E; the small imaginary term $i\epsilon$, $\epsilon \rightarrow 0^+$, serves to make the Green's function

$$G = \frac{1}{E + i\epsilon - K - V} \tag{2}$$

well defined.

Generally it is convenient to think of the operator T as a matrix in the momentum representation with matrix elements denoted by $\langle \vec{k}_2 | T | \vec{k}_1 \rangle$. It is also useful to introduce a complex wave number k, which is related to the total energy by

$$k = \sqrt{\frac{2m}{\hbar^2}(E + i\epsilon)} \qquad [\mathrm{Im}(k) > 0] \tag{3}$$

where m is the reduced mass; thus the energy dependence of the T matrix may be indicated explicitly by writing $\langle \vec{k}_2 | T(k) | \vec{k}_1 \rangle$, or simply $T(k)$.

For most quantum mechanical systems, an expression for the T matrix in closed form cannot be found. The case of a two-particle system with pure Coulomb interaction has been studied extensively, however, and recently Hostler (refs. 1 and 2) has been able to derive an integral representation for the Coulomb Green's function that can be written in terms of hypergeometric functions. From these it is relatively straightforward to obtain the Coulomb T matrix.

The resulting expression for $T(k)$, however, has the drawback that it does not approach a well-defined limit as $k \to \pm|\vec{k}_1|$ or $k \to \pm|\vec{k}_2|$ and indeed has branch points there. This behavior is certainly not correct, for one can show on very general grounds that the only singularities of $T(k)$ should be a branch point at $k = 0$ and simple poles on the imaginary k-axis corresponding to the bound state energies of $K + V$.

The correct form of the T matrix when $k = \pm|\vec{k}_1|$ is given in reference 3, where a similar anomaly in the limiting process $|\vec{k}_2| \to |\vec{k}_1|$ was studied. The difficulty there was traced back to the long-range nature of the Coulomb force and disappeared when the effects of shielding were included.

In the present situation the nonphysical branch points are also due to neglect of shielding effects. In all cases of physical interest, the scattering of charged particles is caused by an interaction which is screened at very large distances. The T matrix may therefore properly be regarded as depending on two parameters, ϵ and the screening radius R. When the value of $T(k)$ for real k is desired, the correct order of limiting processes is $\epsilon \to 0$ followed by $R \to \infty$. Usually, the ordering is unimportant, but the branch points mentioned occur because in Hostler's expression the limit $R \to \infty$ has been (implicitly) taken first.

The purpose of the present work is to clarify the situation, first, by showing that the correct form of $T(k)$ is obtained as $k \to \pm|\vec{k}_1|$ and the branch points disappear if the effects of shielding are taken into account; and, second, by showing that the order of limiting processes is unimportant except in the vicinity of $k = \pm|\vec{k}_1|$ and $k = \pm|\vec{k}_2|$ or when $|\vec{k}_1| = |\vec{k}_2|$. (The last case requires rather special treatment and will not be considered here; in what follows it is assumed that $|\vec{k}_1| \neq |\vec{k}_2|$.)

UNSCREENED COULOMB T MATRIX

In this section an expression for the unscreened Coulomb T matrix which is essentially due to Hostler will be presented. His result for the Green's function for a pure Coulomb potential $V(r) = V_0/r$ is

$$\frac{\hbar^2}{2m}\langle\vec{k}_2|G|\vec{k}_1\rangle = \frac{\delta(\vec{k}_2 - \vec{k}_1)}{k^2 - k_1^2} + \frac{mV_0}{\pi^2\hbar^2}\frac{1 + M}{\left(k^2 - k_1^2\right)\left(k^2 - k_2^2\right)\left(\vec{k}_2 - \vec{k}_1\right)^2} \tag{4}$$

where

$$M = \frac{2i\eta}{e^{-2\pi\eta} - 1}\int_{\infty}^{(1+)}\left(\frac{s - 1}{s + 1}\right)^{i\eta}\frac{1}{\rho^2 - s^2}\,ds \tag{5}$$

$$\rho^2 = 1 + \frac{\left(k^2 - k_1^2\right)\left(k^2 - k_2^2\right)}{k^2(\vec{k}_2 - \vec{k}_1)^2} \tag{6}$$

$$\eta = \frac{mV_0}{\hbar^2 k} \tag{7}$$

From equation (4), the T matrix may be obtained as follows. The operator relation

$$G = \frac{1}{E + i\epsilon - K} + \frac{1}{E + i\epsilon - K}\,T\,\frac{1}{E + i\epsilon - K} \tag{8}$$

becomes, in the momentum representation,

$$\langle\vec{k}_2|G|\vec{k}_1\rangle = \frac{2m}{\hbar^2}\frac{\delta(\vec{k}_2 - \vec{k}_1)}{k^2 - k_1^2} + \left(\frac{2m}{\hbar^2}\right)^2\frac{\langle\vec{k}_2|T|\vec{k}_1\rangle}{\left(k^2 - k_2^2\right)\left(k^2 - k_1^2\right)} \tag{9}$$

If this equation is solved algebraically for the T matrix and equation (4) is used,

$$\langle\vec{k}_2|T|\vec{k}_1\rangle = \frac{V_0}{2\pi^2}\frac{1 + M}{(\vec{k}_2 - \vec{k}_1)^2} \tag{10}$$

The integral M may be evaluated in terms of the hypergeometric function ${}_2F_1$ by changing to

$$x = \frac{s - 1}{s + 1}$$

as the variable of integration, with the result

$$\langle \vec{k}_2 | T | \vec{k}_1 \rangle = \frac{V_0}{2\pi^2} \frac{1}{(\vec{k}_2 - \vec{k}_1)^2} \left\{ 1 + \frac{1}{\rho} \left[{}_2F_1\left(1, i\eta; 1 + i\eta; \frac{\rho + 1}{\rho - 1}\right) \right.\right.$$

$$\left.\left. - {}_2F_1\left(1, i\eta; 1 + i\eta; \frac{\rho - 1}{\rho + 1}\right) \right] \right\} \qquad (11)$$

Considered as a function of k, the right side of equation (11) has simple poles at $i\eta = -n$ ($n = 1, 2, 3 \ldots$) and branch points at $\rho^2 = 1$ and $\rho^2 = \infty$. These latter points correspond to $k = \pm|\vec{k}_1|$, $k = \pm|\vec{k}_2|$, $k = 0$, and $k = \infty$. The detailed behavior of $T(k)$ as $k \to \pm|\vec{k}_1|$ may be determined by analytic continuation of the hypergeometric series and is given by

$$\langle \vec{k}_2 | T(k) | \vec{k}_1 \rangle \to \frac{V_0}{2\pi^2} \frac{\left(k_2^2 - k^2\right)^{i\eta}}{\left[(\vec{k}_2 - \vec{k}_1)^2\right]^{1+i\eta}} \left\{ \frac{2\pi\eta}{1 - e^{-2\pi\eta}} \left(\frac{k_1^2 - k^2}{4k^2}\right)^{i\eta} \right\} \qquad (12)$$

where

$$-\pi < \arg\left(k_2^2 - k^2\right) < 0$$

$$\pi < \arg\left(k_1^2 - k^2\right) < 2\pi$$

(The corresponding result for $k \to \pm|\vec{k}_2|$ is readily obtained from the symmetry of the T matrix with respect to $\vec{k}_1$ and $\vec{k}_2$.) This result is to be contrasted with the exact result of reference 3:

$$\langle \vec{k}_2 | T(k_1) | \vec{k}_1 \rangle = \frac{V_0}{2\pi^2} C_0(\eta) e^{i\delta_0} \frac{\left(k_2^2 - k_1^2\right)^{i\eta}}{\left[(\vec{k}_2 - \vec{k}_1)^2\right]^{1+i\eta}} \qquad (13)$$

Equations (12) and (13) agree in their dependence on k_2^2 and $(\vec{k}_2 - \vec{k}_1)^2$, but they differ in magnitude and phase (C_0 and δ_0 are defined in the next section). In fact, the quantity in braces does not approach a well-defined limit as $k \to \pm|\vec{k}_1|$, and its magnitude may vary by as much as a factor of $e^{\pi\eta}$. For a precise definition of the T matrix in this energy region, the effects of screening must be considered.

SCREENED COULOMB T MATRIX

Ideally, one would like to find the T matrix for some screened Coulomb potential and study its behavior as $R \to \infty$. Then, as discussed in the INTRODUCTION, the Coulomb T matrix could meaningfully be defined as

$$T(k) = \lim_{R \to \infty} T^{(R)}(k)$$

or by a suitable limiting procedure when this limit does not exist. In principle, such a program could be carried out by means of an expansion in spherical harmonics, although it is highly doubtful that the series for $T^{(R)}$ could be summed in closed form. One may conjecture, however, that the series for $T^{(\infty)}$ is summable and in fact is given by Hostler's expression except when $k \to \pm|\vec{k}_1|$ or $k \to \pm|\vec{k}_2|$. Some support for this belief may be found in the fact that equation (12) has the right angular dependence with only its magnitude and phase in doubt.

To establish the conjecture rigorously requires examining the general term in the expansion of $T^{(R)}$ and comparing it to the general term in the expansion of Hostler's result. Here a less ambitious program will be followed, that of comparing only the $\ell = 0$ terms. A qualitative investigation of the terms for $\ell > 0$, however, will also be made.

Expansion in Spherical Harmonics

In order to parallel the treatment of reference 3, delta-function normalization for the wave functions will be adopted, and the expansion of the T matrix will be written in the form

$$\langle \vec{k}_2|T|\vec{k}_1\rangle = -\frac{\hbar^2}{4\pi^2 m}\sum_{\ell=0}^{\infty}(2\ell + 1)P_\ell(\hat{k}_2 \cdot \hat{k}_1)\langle k_2|T_\ell|k_1\rangle \tag{14}$$

where

$$\langle k_2 | T_\ell | k_1 \rangle = -\frac{2\pi^2 m}{\hbar^2} \int_{-1}^{1} \langle \vec{k}_2 | T | \vec{k}_1 \rangle P_\ell(\mu) d\mu \qquad (\mu = \hat{k}_2 \cdot \hat{k}_1) \tag{15}$$

and $P_\ell(\mu)$ is a Legendre polynomial of order ℓ.

The coefficients $T_\ell(k)$ for an arbitrary potential $V(r)$ may be obtained from equations (1) and (15) if the corresponding Green's function is known. This is accomplished by making an expansion of the coordinate representation of the Green's function:

$$\langle \vec{r} | G | \vec{r}' \rangle = \frac{2m}{\hbar^2} \sum_{\ell=0}^{\infty} \left(\frac{2\ell + 1}{4\pi} \right) P_\ell(\hat{r} \cdot \hat{r}') \langle r | G_\ell | r' \rangle \tag{16}$$

After the angular integrations are carried out,

$$\langle k_2 | T_\ell | k_1 \rangle = -\int_0^\infty j_\ell(k_2 r) W(r) j_\ell(k_1 r) r^2 \, dr$$

$$- \int_0^\infty r^2 \, dr \int_0^\infty r'^2 \, dr' \, j_\ell(k_2 r) W(r) \langle r | G_\ell | r' \rangle W(r') j_\ell(k_1 r') \tag{17}$$

where $W(r) = (2m/\hbar^2)V(r)$ and $j_\ell(kr)$ is a spherical Bessel function of order ℓ.

To obtain $\langle r | G_\ell | r' \rangle$, the operator equation

$$(E + i\epsilon - K - V)G = 1 \tag{18}$$

is written in the coordinate representation, from which it follows that

$$\left[\frac{1}{r} \frac{d^2}{dr^2} r + k^2 - \frac{\ell(\ell + 1)}{r^2} - W(r) \right] \langle r | G_\ell | r' \rangle = \frac{\delta(r - r')}{r^2} \tag{19}$$

The solution to this equation is well known to be

$$\langle r | G_\ell | r' \rangle = \frac{1}{ikrr'} F_\ell(r_<) H_\ell(r_>) \tag{20}$$

where $r_<$ is the smaller and $r_>$ the larger of r, r', and where F_ℓ and H_ℓ are the regular and irregular solutions of

$$\left[\frac{d^2}{dr^2} + k^2 - \frac{\ell(\ell+1)}{r^2} - W(r)\right] u_\ell(r) = 0 \tag{21}$$

having the asymptotic forms

$$F_\ell(r) \sim \sin\left(kr - \frac{1}{2}\pi\ell + \delta_\ell\right)$$

$$H_\ell(r) \sim -ie^{i\left(kr - \frac{1}{2}\pi\ell + \delta_\ell\right)} \tag{22}$$

The phase shift δ_ℓ is determined by the fact that $F_\ell(r)$ must vanish at $r = 0$, and the normalization is so chosen that the Wronskian of F_ℓ and H_ℓ is equal to ik.

By combining equations (17) and (20), one may write

$$\langle k_2 | T_\ell | k_1 \rangle = -I_\ell - J_\ell \tag{23}$$

where

$$I_\ell = \int_0^\infty j_\ell(k_2 r) W(r) j_\ell(k_1 r) r^2 \, dr \tag{24}$$

and where

$$J_\ell = J_\ell(12) + J_\ell(21)$$

$$J_\ell(12) = \frac{1}{ik}\int_0^\infty j_\ell(k_2 r) W(r) F_\ell(r) \int_r^\infty j_\ell(k_1 r') W(r') H_\ell(r') r' \, dr' \, r \, dr \tag{25}$$

and $J_\ell(21)$ is identical to $J_\ell(12)$ except that k_1 and k_2 are interchanged.

Cutoff Coulomb Wave Functions

The simplest way to screen the Coulomb field is to cut it off at $r = R$, so that the potential is

$$
\begin{aligned}
V(r) &= V_0/r \qquad && (r < R) \\
&= 0 && (r > R)
\end{aligned}
\tag{26}
$$

The solutions of equation (21) here must be proportional to pure Coulomb functions for $r < R$ and to free-particle functions for $r > R$. The free-particle functions are so chosen that the asymptotic forms of equation (22) are obtained for large r. Thus,

$$
\left.
\begin{aligned}
\frac{F_\ell(r)}{kr} &= N_\ell (2kr)^\ell e^{ikr} \Phi(\ell + 1 + i\eta,\ 2\ell + 2;\ -2ikr) \qquad && (r < R) \\
\frac{F_\ell(r)}{kr} &= \frac{1}{2}\left[e^{i\delta_\ell} h_\ell^{(1)}(kr) + e^{-i\delta_\ell} h_\ell^{(2)}(kr)\right] && (r > R)
\end{aligned}
\right\}
\tag{27}
$$

$$
\left.
\begin{aligned}
\frac{H_\ell(r)}{kr} &= N_\ell' (2kr)^\ell e^{ikr} \Psi(\ell + 1 + i\eta,\ 2\ell + 2;\ -2ikr) \qquad && (r < R) \\
\frac{H_\ell(r)}{kr} &= e^{i\delta_\ell} h^{(1)}(kr) && (r > R)
\end{aligned}
\right\}
\tag{28}
$$

where Φ and Ψ are confluent hypergeometric functions (ref. 4), and $h_\ell^{(1)}$ and $h_\ell^{(2)}$ are spherical Hankel functions of the first and second kind of order ℓ.

The constants N_ℓ and δ_ℓ may be determined by equating logarithmic derivatives of F_ℓ at $r = R$; approximate values for large R are (ref. 3)

$$
N_\ell \sim C_\ell(\eta) \qquad \delta_\ell \sim \sigma_\ell - \eta \ln(2kR) \tag{29}
$$

where

$$
C_\ell(\eta) = e^{-\frac{1}{2}\pi\eta - i\sigma_\ell} \frac{\Gamma(\ell + 1 + i\eta)}{\Gamma(2\ell + 2)} \tag{30}
$$

$$e^{2i\sigma_\ell} = \frac{\Gamma(\ell + 1 + i\eta)}{\Gamma(\ell + 1 - i\eta)} \tag{31}$$

An exact value for the product $N_\ell N'_\ell$ will be necessary and can be obtained from the fact that the Wronskian of F_ℓ and H_ℓ must be equal to ik. After some algebra, one finds that

$$F_\ell H'_\ell - F'_\ell H_\ell = \frac{kN_\ell N'_\ell \Gamma(2\ell + 2)}{2i\Gamma(\ell + 1 + i\eta)} (-1)^\ell = ik$$

which yields

$$N_\ell N'_\ell = 2(-1)^{\ell+1} \frac{\Gamma(\ell + 1 + i\eta)}{\Gamma(2\ell + 2)} = 2(-1)^{\ell+1} e^{\frac{1}{2}\pi\eta + i\sigma_\ell} C_\ell(\eta) \tag{32}$$

Finally, from the integral representations of Φ and Ψ, the following expressions (valid for $r < R$) can be derived:

$$W(r)F_0(r) = -\frac{k^2 N_0}{2\pi} \oint \left(\frac{t + 1}{t - 1}\right)^{i\eta} e^{-ikrt}\, dt \tag{33}$$

$$W(r)H_0(r) = -\frac{k^2 N'_0}{2\pi} e^{\pi\eta}\, \Gamma(1 - i\eta) \int_\infty^{(+1)} \left(\frac{s - 1}{s + 1}\right)^{i\eta} e^{ikrs}\, ds \tag{34}$$

The t-contour is a loop encircling the points $t = \pm 1$ in the positive sense; the phases are such that $\arg(t \pm 1) = 0$ when t crosses the real axis to the right of $t = 1$. The s-contour is a "loop" which begins at $s = \infty$, encircles the point $s = 1$ in the positive sense, and returns to $s = \infty$; the phases are such that initially $\arg(s \pm 1) = 0$.

Evaluation of $T_0(k)$

For the cutoff Coulomb potential, the integral I_0 becomes

$$I_0 = \frac{2\eta k}{k_1 k_2} \int_0^R \sin k_2 r \sin k_1 r \frac{dr}{r}$$

$$= \frac{\eta k}{k_1 k_2} \left\{ \ln \frac{k_1 + k_2}{|k_1 - k_2|} + \mathrm{Ci}\left[|k_1 - k_2| R\right] - \mathrm{Ci}\left[(k_1 + k_2) R\right] \right\} \tag{35}$$

where $\mathrm{Ci}(x)$ is the cosine integral (ref. 3, p. 267). Since the case $k_1 = k_2$ is not being considered here,

$$I_0 = \frac{\eta k}{k_1 k_2} \ln \frac{k_1 + k_2}{|k_1 - k_2|} + \mathcal{O}\left(\frac{1}{R}\right) \tag{36}$$

To evaluate J_0, it is convenient to express $\sin(k_2 r)$ and $\sin(k_1 r')$ in terms of exponentials and to introduce the integral representations (33) and (34). Then J_0 can be written as the sum of four integrals of the type

$$A = Q \int_\infty^{(1+)} \left(\frac{s-1}{s+1}\right)^{i\eta} \oint \left(\frac{t+1}{t-1}\right)^{i\eta} B \, dt \, ds \tag{37}$$

where $B = B(12) + B(21)$ and

$$B(12) = -\int_0^R e^{-ir(kt+k_2)} \int_r^R e^{ir'(ks-k_1)} \, dr' \, dr \tag{38}$$

$$Q = \frac{k^3 N_0 N_0'}{16\pi^3 i} e^{\pi\eta} \Gamma(1 - i\eta) = -\frac{\eta k^3}{4\pi i} \left(1 - e^{-2\pi\eta}\right)^{-1} \tag{39}$$

Specifically,

$$J_0 = \frac{1}{k_1 k_2} \left[A(k_1, k_2) - A(k_1, -k_2) - A(-k_1, k_2) + A(-k_1, -k_2)\right] \tag{40}$$

The integral for B(12) is easily carried out and finally leads to

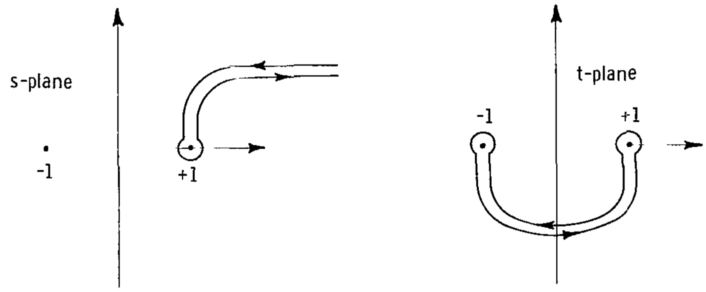

Figure 1. - Integration contours for confluent hypergeometric functions.

$$B = \frac{\alpha + \tilde{\alpha}}{\alpha\tilde{\alpha}(\alpha - \beta)} + \frac{e^{i\alpha R}}{\alpha\beta} + \frac{e^{i\tilde{\alpha}R}}{\tilde{\alpha}\tilde{\beta}} - \frac{\beta + \tilde{\beta}}{\beta\tilde{\beta}(\alpha - \beta)} e^{i(\alpha-\beta)R} \tag{41}$$

where

$$\left.\begin{aligned} \alpha &= ks - k_1 \\ \beta &= kt + k_2 \end{aligned}\right\} \tag{42}$$

and $\tilde{\alpha}$ and $\tilde{\beta}$ are the corresponding quantities with k_1 and k_2 interchanged. Since B has no singularities for finite s and t, the contours may be deformed as desired; deforming them as shown in figure 1 is convenient because then the singularities of the individual terms in B do not cross the contours as $\mathrm{Im}(k) \to 0$.

The roles of the four terms in B are as follows. Generally the main contribution is from the first term, the others being of order $1/R$. When $k \to k_1$, however, the second term cancels part of the first and makes a contribution of its own. A similar remark holds for the third term when $k \to k_2$. It may be shown (see appendix) that the fourth term is always negligible provided that $k_1 \neq k_2$; this term will not be considered further. Thus in an obvious notation

$$A = A_1 + A_2 + A_3 + \mathcal{O}\left(\frac{1}{R}\right) \tag{43}$$

and, correspondingly,

$$J_0 = J_0' + J_0'' + J_0''' + \mathcal{O}\left(\frac{1}{R}\right) \tag{44}$$

The t-integration for A_1 is performed by expanding the contour into a circle of infinite radius, which yields

$$\oint \left(\frac{t+1}{t-1}\right)^{i\eta} \frac{dt}{\alpha - \beta} = \frac{2\pi i}{k}\left[\left(\frac{s-\nu+1}{s-\nu-1}\right)^{i\eta} - 1\right] \tag{45}$$

where $\nu = (k_1 + k_2)/k$. Then A_1 can be written in the form

$$A_1 = 2\pi i Q \lim_{L \to \infty} \int_L^{(+1)} \left(\frac{s-1}{s+1}\right)^{i\eta}\left[\left(\frac{s-\nu+1}{s-\nu-1}\right)^{i\eta} - 1\right] \frac{2s-\nu}{(ks-k_1)(ks-k_2)}\, ds \tag{46}$$

Actually the integral is convergent even when $L = \infty$, but the limiting process allows A_1 to be considered as the difference of two otherwise divergent integrals, which may thus be treated separately. In the first of these integrals, let

$$x = \frac{(L+1)(L-\nu-1)(s-1)(s-\nu+1)}{(L-1)(L-\nu+1)(s+1)(s-\nu-1)}$$

and in the second let

$$y = \frac{(L+1)(s-1)}{(L-1)(s+1)}$$

Then, after some manipulation, A_1 may be written

$$A_1 = \frac{2\pi i Q}{k^2} \lim_{L \to \infty}\left[a^{i\eta}\int_1^{(0+)} x^{i\eta}\left(\frac{a}{1-ax} - \frac{auv}{1-auvx}\right) dx \right.$$

$$\left. - b^{i\eta}\int_1^{(0+)} y^{i\eta}\left(\frac{2b}{1-by} - \frac{bu}{1-buy} - \frac{bv}{1-bvy}\right) dy\right] \tag{47}$$

where

$$\left.\begin{aligned} a &= \frac{(L-1)(L-\nu+1)}{(L+1)(L-\nu-1)} \\ b &= \frac{L-1}{L+1} \end{aligned}\right\} \tag{48}$$

$$
\left.
\begin{aligned}
u &= \frac{k_1 + k}{k_1 - k} \\
v &= \frac{k_2 + k}{k_2 - k}
\end{aligned}
\right\} \tag{49}
$$

The integrals in equation (47) are all of the same general type, being integral representations of a function here denoted by $D(x)$:

$$
\begin{aligned}
D(x) &\equiv \left(e^{-2\pi\eta} - 1\right)^{-1} \int_1^{(0+)} t^{i\eta} \frac{x}{1 - xt}\, dt \\
&= \frac{1}{1 + i\eta}\, x \; {}_2F_1(1, 1 + i\eta;\; 2 + i\eta;\; x)
\end{aligned} \tag{50}
$$

Therefore

$$
A_1 = \frac{1}{2} \eta k \lim_{L \to \infty} \left\{ a^{i\eta} \left[D(a) - D(auv) \right] - b^{i\eta} \left[2D(b) - D(bu) - D(bv) \right] \right\} \tag{51}
$$

From the analytic continuation of the hypergeometric function,

$$
D(x) \xrightarrow[x \to 1]{} \psi(1 + i\eta) - \psi(1) - \ln(1 - x) \qquad \left|\arg(1 - x)\right| < \pi \tag{52a}
$$

$$
D(x) \xrightarrow[x \to \infty]{} \frac{1}{i\eta} \left[e^{2\pi\eta} C_0(\eta)^2 \left(\frac{1}{x}\right)^{i\eta} - 1 \right] \qquad 0 < \arg\left(\frac{1}{x}\right) < 2\pi \tag{52b}
$$

where $\psi(x)$ is the logarithmic derivative of the gamma function. The limit $L \to \infty$ may be taken with the help of equation (52a), and after the combination of equation (40) is performed

$$
\begin{aligned}
J_0^{*} = &- \frac{\eta k}{k_1 k_2} \ln \frac{k_1 + k_2}{\left|k_1 - k_2\right|} \\
&- \frac{\eta k}{2 k_1 k_2} \left[D(uv) - D\left(\frac{u}{v}\right) - D\left(\frac{v}{u}\right) + D\left(\frac{1}{uv}\right) \right]
\end{aligned} \tag{53}
$$

Note that the first term in J_0', which arises from the limiting value of $D(a) - 2D(b)$, is just equal to $-I_0$.

When $k \to k_1$, the expression for J_0' simplifies because the arguments of D approach either zero or infinity. From equations (50) and (52b) it follows that

$$J_0' \xrightarrow[k \to k_1]{} - I_0 - \frac{e^{2\pi\eta} C_0(\eta)^2}{2ik_2} \left[\left(\frac{1}{uv}\right)^{i\eta} - \left(\frac{v}{u}\right)^{i\eta}\right] \tag{54}$$

with the phases of both $1/uv$ and v/u between 0 and 2π.

The t-integration for A_2 is carried out as for A_1 and leads to

$$A_2 = \frac{2\pi i Q}{k^2}\left[1 - \left(\frac{k_2 - k}{k_2 + k}\right)^{i\eta}\right] f(k_1) \tag{55}$$

where

$$f(k_1) = e^{-ik_1R} \int_{\infty}^{(1+)} \left(\frac{s - 1}{s + 1}\right)^{i\eta} \frac{e^{ikRs}}{s - k_1/k}\, ds \tag{56}$$

The expression for J_0'' then takes the form

$$J_0'' = \frac{2\pi i Q}{k^2 k_1 k_2}\left[v^{i\eta} - \left(\frac{1}{v}\right)^{i\eta}\right]\left[f(k_1) - f(-k_1)\right] \tag{57}$$

From the way in which the t contour is laid, one can show that both $\arg(1/v)$ and $\arg(v)$ must be approximately between $-3\pi/2$ and $\pi/2$.

The integral in equation (56) is generally of order $1/R$, as may be demonstrated by integrating by parts. This argument fails, however, when $k \to k_1$, because the contour must pass between the singularities at $s = 1$ and $s = k_1/k$, and these singularities merge in the limit. The difficulty may be avoided by first enlarging the contour so that it also encloses the pole at $s = k_1/k$:

$$f(k_1) = -2\pi i\left(\frac{k_1 - k}{k_1 + k}\right)^{i\eta} + e^{-ik_1R} \int_{\Gamma} \left(\frac{s - 1}{s + 1}\right)^{i\eta} \frac{e^{ikRs}}{s - k_1/k}\, ds \tag{58}$$

The contour Γ is now such that, for sufficiently small $|k - k_1|$, the factor $(s - k_1/k)^{-1}$ may be expanded about $s = 1$ and term-by-term integration performed. The resulting integrals may be recognized as confluent hypergeometric functions, and to lowest order

$$f(k_1) = -2\pi i\left[\left(\frac{1}{u}\right)^{i\eta} - \frac{e^{-\pi\eta}}{\Gamma(1 - i\eta)}\,\Psi(i\eta, 1;\; -2ikR)\right] + \mathcal{O}\left[(k - k_1)R\right] \tag{59}$$

From the derivation it is clear that $0 \leq \arg(1/u) \leq 2\pi$, and since k_1 is positive, this becomes $\pi \leq \arg(1/u) \leq 2\pi$. For large R, the asymptotic form of Ψ may be used to write

$$f(k_1) = -2\pi i\left[\left(\frac{1}{u}\right)^{i\eta} - \frac{e^{-\frac{3}{2}\pi\eta}}{\Gamma(1 - i\eta)}(2kR)^{-i\eta}\right] + \mathcal{O}\left(\frac{1}{R}\right) + \mathcal{O}\left[(k - k_1)R\right] \tag{60}$$

Two things are noteworthy here. First, there is the appearance of the logarithmic phase factor $(2kR)^{-i\eta}$, known to be necessary when $k \to |k_1|$ from the work of reference 3. Second, the order of magnitude estimates of the neglected terms in equation (60) show clearly that this result can be achieved only if the order of limits is $k \to k_1$ followed by $R \to \infty$.

Through use of the definitions of $C_0(\eta)$ and δ_0, the final result for J_0'' when $k \to k_1$ may be expressed as

$$J_0'' \to -\frac{C_0(\eta)e^{i\delta_0}}{2ik_2}\left[\left(\frac{1}{v}\right)^{i\eta} - v^{i\eta}\right] + \frac{e^{2\pi\eta}C_0(\eta)^2}{2ik_2}\left[\left(\frac{1}{uv}\right)^{i\eta} - \left(\frac{v}{u}\right)^{i\eta}\right] + \mathcal{O}\left(\frac{1}{R}\right) \tag{61}$$

A similar treatment may be made when $k \to -k_1$; for all other values of k, $J_0'' = \mathcal{O}(1/R)$. Finally, examination of the third term in B (eq. (41)) shows that J_0''' is identical to J_0'' except that k_1 and k_2 are interchanged. Thus the evaluation of J_0 to order $1/R$ is complete, and $T_0(k)$ may be determined.

In the general case, where only J_0' is nonvanishing for large R,

$$\langle k_2|T_0|k_1\rangle = \frac{\eta k}{2k_1k_2}\left[D\left(\frac{1}{uv}\right) - D\left(\frac{u}{v}\right) - D\left(\frac{v}{u}\right) + D(uv)\right] \tag{62}$$

in the limit $R \to \infty$. This equation corresponds exactly to Hostler's result, as will be shown in a later section. In particular, there are branch points at $k = \pm k_1$ and $k = \pm k_2$. Clearly, however, these branch points do not appear if the limit $R \to \infty$ is taken last.

Consider the case $k \to k_1$; here both J_0' and J_0'' are important, and when equations (54) and (61) are combined

$$\langle k_2 | T_0 | k_1 \rangle \to \frac{C_0(\eta) e^{i\delta_0}}{2ik_2} \left[\left(\frac{1}{v}\right)^{i\eta} - v^{i\eta} \right] + \mathcal{O}\left(\frac{1}{R}\right) \tag{63}$$

The limiting value of T_0 is independent of the way in which $k \to k_1$ and, in view of the restrictions on $\arg(1/v)$ and $\arg(v)$, may be written

$$\langle k_2 | T_0(k_1) | k_1 \rangle = \frac{C_0(\eta) e^{i\delta_0}}{2ik_2} \left\{ \left| \frac{k_2 - k_1}{k_2 + k_1} \right|^{i\eta} - \left| \frac{k_2 + k_1}{k_2 - k_1} \right|^{i\eta} \right\} \times \begin{Bmatrix} 1 \\ e^{\pi\eta} \end{Bmatrix} + \mathcal{O}\left(\frac{1}{R}\right)$$

$$\text{for} \begin{Bmatrix} k_2 > k_1 \\ k_2 < k_1 \end{Bmatrix} \tag{64}$$

This is identical to the result found in reference 3.

PROPERTIES OF $T_\ell(k)$

Although no detailed investigation of T_ℓ has been made for higher values of ℓ, reasonable predictions about what to expect are not difficult to make. For higher ℓ values in the shielded case, $j_\ell(k_1 r')$ and $j_\ell(k_2 r)$ would be written in terms of spherical Hankel functions; this would again lead naturally to four J_ℓ integrals, of which only the first would be independent of R. Presumably the other three would be of order $1/R$ except in the vicinity of the branch points, as in the $\ell = 0$ case. It is not unreasonable, then, to suppose that the R-independent term is the same one that would be obtained for the unscreened potential, and therefore that the screened and unscreened T matrices are identical in the limit $R \to \infty$ save for the exceptional points.

To strengthen this argument, consider the integral

$$ikJ_\ell(12) = \int_0^R \omega_1(r) \int_r^R \omega_2(r')\, dr'\, dr \tag{65}$$

which arises in the calculation of T_ℓ. Here

$$\omega_1(r) = rj_\ell(k_2r)W(r)F_\ell(r) \qquad (r < R)$$

$$\omega_2(r) = rj_\ell(k_1r)W(r)H_\ell(r) \qquad (r < R) \tag{66}$$

and because r and r' are always less than R, F_ℓ and H_ℓ are pure Coulomb functions.

Now the integral in equation (65) may be rewritten

$$ikJ_\ell(12) = \int_0^\infty \omega_1(r) \int_r^\infty \omega_2(r')dr'\, dr - \left[\int_0^\infty \omega_1(r)dr\right]\left[\int_R^\infty \omega_2(r)dr\right]$$

$$- \int_R^\infty \omega_1(r) \int_r^\infty \omega_2(r')dr'\, dr \tag{67}$$

provided that ω_1 and ω_2 are given some suitable definition for $r > R$. For the present purpose, it is convenient to require that ω_1 and ω_2 have the <u>same functional form</u> for $r > R$ as for $r < R$, that is, ω_1 and ω_2 are proportional to pure Coulomb functions multiplied by spherical Bessel functions for <u>all</u> r.

With this definition, it is clear that the first term in equation (67) is just what one would write for the unscreened Coulomb potential. The second term is similar to J_0'' of the preceding section in that it factors into a function of k_2 multiplied by a function of k_1. Regarding the second factor, one can show that

$$\int_R^\infty \omega_2(r)dr = e^{ikR}\,\mathcal{O}\left[\frac{1}{\left(k^2 - k_1^2\right)R}\right] \tag{68}$$

This follows from the fact that for large values of r,

$$\omega_2(r) \sim \eta k N_\ell' i^{\ell+1+i\eta} \frac{\sin\left(k_1r - \frac{1}{2}\pi\ell\right)}{k_1r} \frac{e^{ikr}}{(2kr)^{i\eta}} \tag{69}$$

The rapid oscillations of the exponentials make the integral small unless $k \to \pm k_1$. In like manner, by using the asymptotic forms of ω_1 and ω_2, one may show (see appendix) that the third integral in equation (67) is of order $1/R$ unless both $k \to \pm k_1$ and $k \to \pm k_2$, which is possible only if $|k_1| = |k_2|$.

These findings reveal that $J_\ell(12)$ departs from its unscreened value only when contributions to the integral from large r are important, and these contributions occur only when $k \to \pm k_1$. Similar conclusions may be drawn for $J_\ell(21)$, the critical condition becoming $k \to \pm k_2$. Thus,

$$J_\ell^{(R)} = J_\ell^{(\infty)} + \mathcal{O}\left[\frac{1}{\left(k^2 - k_1^2\right)R}\right] + \mathcal{O}\left[\frac{1}{\left(k^2 - k_2^2\right)R}\right] \tag{70}$$

To complete the investigation of T_ℓ, the behavior of I_ℓ as $R \to \infty$ must be determined. The subtraction procedure used above is also effective here, and leads easily to

$$I_\ell^{(R)} = I_\ell^{(\infty)} + \mathcal{O}\left[\frac{1}{\left(k_1 - k_2\right)R}\right] \tag{71}$$

From this and equation (70), it follows that

$$T^{(R)} = T^{(\infty)} + \mathcal{O}\left[\frac{1}{\left(k \pm k_1\right)R}\right] + \mathcal{O}\left[\frac{1}{\left(k \pm k_2\right)R}\right] + \mathcal{O}\left[\frac{1}{\left(k_1 - k_2\right)R}\right] \tag{72}$$

which is the desired result.

It is instructive to examine the way in which T_ℓ changes as the contributions from large r come into play. Consider the case $k \to k_1$; from equation (69) and the fact that

$$N_\ell' \sim 2(-1)^{\ell+1} e^{\pi\eta/2} e^{i\sigma_\ell}$$

and

$$\delta_\ell \sim \sigma_\ell - \eta \ln(2kR)$$

as $R \to \infty$,

$$\int_R^\infty \omega_2(r)dr = \frac{\eta k}{k_1} R^{i\eta} e^{i\delta_\ell} \int_R^\infty e^{-i(k_1-k)r} \frac{dr}{r^{1+i\eta}} + \mathcal{O}\left(\frac{1}{R}\right) \tag{73}$$

This integral may be evaluated from the formula

$$R^{i\eta}\int_R^\infty e^{-\lambda r}\,\frac{dr}{r^{1+i\eta}} = e^{-\lambda R}\,\Psi(1, 1 - i\eta;\ \lambda R) \qquad \left(|\arg(\lambda)| < 1/2\ \pi\right)$$

$$= \frac{1}{i\eta}\left[e^{-\lambda R}\,\Phi(1, 1 - i\eta;\ \lambda R) - (\lambda R)^{i\eta}\,\Gamma(1 - i\eta)\right] \tag{74}$$

The lower form of equation (74) is appropriate to the present case, which corresponds to $R \to \infty$, $\lambda R \to 0$. Because of the restriction on $\arg(\lambda)$,

$$\left(\frac{\lambda}{2k}\right)^{i\eta} = \left[\frac{i(k_1 - k)}{2k}\right]^{i\eta}$$

$$= e^{\frac{3}{2}\pi\eta}\left(\frac{1}{u}\right)^{i\eta} + \mathcal{O}(k - k_1) \qquad \pi \leq \arg\left(\frac{1}{u}\right) \leq 2\pi \tag{75}$$

Then, since $\Phi(x) \to 1$ as $x \to 0$,

$$\int_R^\infty \omega_2(r)dr = -ie^{i\delta_\ell} + ie^{2\pi\eta}C_0(\eta)e^{i(\sigma_\ell - \sigma_0)}\left(\frac{1}{u}\right)^{i\eta} + \mathcal{O}\left[(k - k_1)R\right] + \mathcal{O}\left(\frac{1}{R}\right) \tag{76}$$

It will now be shown that

$$\int_0^R \omega_1(r)dr = -ke^{-i\delta_\ell}\,\langle k_2|T_\ell(k)|k\rangle \tag{77}$$

that is, the integral is proportional to $T_\ell(k)$ for the special case when k_1 is complex and equal to k. For the proof, it is necessary to consider a "plane wave" $\varphi_{\vec{k}}$ whose wave number is complex:

$$\left.\begin{aligned} \varphi_{\vec{k}}(\vec{r}) &= (2\pi)^{-\frac{3}{2}}\sum_{\ell=0}^{\infty} i^\ell(2\ell + 1)P_\ell(\hat{k}\cdot\hat{r})j_\ell(kr) \\ \frac{\hbar^2k^2}{2m} &= E + i\epsilon \end{aligned}\right\} \tag{78}$$

When the scattering operator T(k) is applied to this function, the result may be expressed as

$$T(k)\varphi_{\vec{k}} = V(r)\psi_{\vec{k}}(\vec{r}) \tag{79}$$

where

$$\psi_{\vec{k}}(\vec{r}) = (1 + GV)\varphi_{\vec{k}}$$

$$= \left(1 + \frac{1}{E + i\epsilon - K - V} V\right)\varphi_{\vec{k}} \tag{80}$$

Thus the T matrix may be written

$$\langle \vec{k}_2 | T(k) | \vec{k} \rangle = (2\pi)^{-3/2} \int e^{-i\vec{k}_2 \cdot \vec{r}} V(r)\psi_{\vec{k}}(\vec{r})d\vec{r} \tag{81}$$

The reason for introducing $\varphi_{\vec{k}}$ becomes clear when one looks for a way to determine $\psi_{\vec{k}}$. Since $\varphi_{\vec{k}}$ is annihilated by the operator $E + i\epsilon - K$, it follows from equation (80) that

$$(E + i\epsilon - K - V)\psi_{\vec{k}} = 0 \tag{82}$$

Thus $\psi_{\vec{k}}$ is an eigenfunction of $K + V$ belonging to the complex energy $E + i\epsilon$, and well-known scattering theory techniques lead to the expansion

$$\psi_{\vec{k}}(\vec{r}) = (2\pi)^{-3/2} \sum_{\ell=0}^{\infty} i^{\ell}(2\ell + 1)P_{\ell}(\hat{k} \cdot \hat{r})e^{i\delta_{\ell}} \frac{F_{\ell}(kr)}{kr} \tag{83}$$

The angular integration in equation (81) may now be carried out and yields

$$\langle \vec{k}_2 | T(k) | \vec{k} \rangle = \frac{\hbar^2}{4\pi^2 m} \sum_{\ell=0}^{\infty} (2\ell + 1)P_{\ell}(\hat{k}_2 \cdot \hat{k})e^{i\delta_{\ell}} \int_0^{\infty} j_{\ell}(k_2 r)W(r) \frac{F_{\ell}(kr)}{kr} r^2\, dr \tag{84}$$

When this equation is compared with equation (14) with the cutoff Coulomb potential for V(r), the result given in equation (77) is obtained.

One final point remains to be made. In equation (77) the upper limit cannot be extended to infinity for arbitrary complex k, because the integral will diverge. It can be shown, however, that

$$\int_0^R \omega_1(r)dr \to g_\ell(k_2, k_1) \qquad \text{as} \begin{cases}(k - k_1)R \to 0 \\ R \to \infty\end{cases} \tag{85}$$

where $g_\ell(k_2, k_1)$ is a finite, well-behaved function provided that $k_1 \neq k_2$. Combining all these results yields

$$\left(\int_0^R \omega_1(r)dr\right)\left(\int_R^\infty \omega_2(r)dr\right) = ik\langle k_2 | T_\ell^{(R)}(k) | k\rangle$$

$$+ ie^{2\pi\eta}C_0(\eta)e^{i(\sigma_\ell - \sigma_0)}g_\ell(k_2, k_1)\left(\frac{1}{u}\right)^{i\eta} + \mathcal{O}\left[(k - k_1)R\right] + \mathcal{O}\left(\frac{1}{R}\right) \tag{86}$$

The first term on the right side is R-dependent through the phase factor $e^{i\delta_\ell}$, and provides the correct definition of T_ℓ as $k \to k_1$. The second term is independent of R and has a branch point at $k = k_1$; clearly its function is to cancel a similar quantity from $J_\ell^{(\infty)}$. This can be seen quite easily in the $\ell = 0$ case, since $J_\ell^{(\infty)} = J_0'$ of the preceding section. Hence,

$$J_0^{(R)} = J_0' - \langle k_2 | T_0^{(R)} | k\rangle - \frac{e^{2\pi\eta}C_0(\eta)}{k_1}\left(\frac{1}{u}\right)^{i\eta} g_0(k_2, k_1) + \mathcal{O}\left[(k - k_1)R\right] + \mathcal{O}\left(\frac{1}{R}\right) \tag{87}$$

From equations (85), (77), and (63), it follows that

$$g_0(k_2, k_1) = -\frac{k_1 C_0(\eta)}{2ik_2}\left[\left(\frac{1}{v}\right)^{i\eta} - v^{i\eta}\right] \tag{88}$$

and thus, using equation (54) for J_0' gives

$$J_0^{(R)} = -I_0 - \langle k_2 | T_0^{(R)} | k\rangle + \mathcal{O}\left[(k - k_1)R\right] + \mathcal{O}\left(\frac{1}{R}\right) \tag{89}$$

The preceding discussion indicates that $J_\ell^{(\infty)}$ may be written as $-I_\ell^{(\infty)}$ plus a term to be cancelled by contributions from large r. Examination of equation (76) reveals that this cancellation is equivalent to replacing

$$ie^{2\pi\eta} C_0(\eta) e^{i(\sigma_\ell - \sigma_0)} \left(\frac{1}{u}\right)^{i\eta}$$

by

$$ie^{i\delta_\ell}$$

as a factor in the term to be cancelled. Since

$$\delta_\ell = \delta_0 + (\sigma_\ell - \sigma_0)$$

the ℓ dependence of $J_\ell^{(\infty)}$ is not affected by this replacement, and

$$T_\ell^{(R)} = \frac{e^{i\delta_0 - 2\pi\eta}}{C_0(\eta)} u^{i\eta} T_\ell^{(\infty)} + \mathcal{O}\left(\frac{1}{R}\right) \qquad \text{as } (k - k_1)R \to 0 \tag{90}$$

The importance of this result is that the angular dependence of $T^{(R)}$ will be the same as that of $T^{(\infty)}$ in the limit $k \to k_1$, and thus from equation (12),

$$\langle \vec{k}_2 | T^{(R)} | \vec{k}_1 \rangle = \frac{V_0}{2\pi^2} C_0(\eta) e^{i\delta_0} \frac{\left(k_2^2 - k^2\right)^{i\eta}}{\left[(\vec{k}_2 - \vec{k}_1)^2\right]^{1+i\eta}} + \mathcal{O}\left(\frac{1}{R}\right) \qquad \text{as } (k - k_1)R \to 0 \tag{91}$$

This result agrees with the findings of reference 3 and in the limit yields equation (13).

CLOSED FORM FOR $T^{(\infty)}(k)$

In the foregoing section, it was more or less tacitly assumed that $T^{(\infty)}(k)$ is given by Hostler's formula provided that k is off the real axis. A study of Hostler's derivation indicates that this is true, since he begins with the same Green's function integrals except that the upper limit is ∞ instead of R. One can also verify directly that $\langle k_2 | T_0 | k_1 \rangle$ is the same for both by evaluating

$$\langle k_2 | T_0 | k_1 \rangle = -\eta k \int_{-1}^{1} \frac{1 + M}{(\vec{k}_2 - \vec{k}_1)^2} \, d\mu \qquad (\mu = \hat{k}_1 \cdot \hat{k}_2) \tag{92}$$

An expression for $1 + M$ is given in equation (11), but a more convenient one for integration purposes is

$$1 + M = \frac{1}{4(1 + i\eta)} \, \frac{\rho^2 - 1}{\rho} \left[{}_2F_1\left(1, 2;\ 2 + i\eta;\ \frac{1 - \rho}{2}\right) - {}_2F_1\left(1, 2;\ 2 + i\eta;\ \frac{1 + \rho}{2}\right) \right] \tag{93}$$

which may be obtained from equation (11) by making use of the transformation properties of the hypergeometric function. Then, since

$$\frac{d\rho}{d\mu} = \frac{k_1 k_2}{(\vec{k}_2 - \vec{k}_1)^2} \, \frac{\rho^2 - 1}{\rho} \tag{94}$$

and

$$\frac{1}{1 + i\eta} \int {}_2F_1\,(1, 2;\ 2 + i\eta;\ x)\, dx = -D\left(\frac{x}{x - 1}\right) \tag{95}$$

where $D(x)$ is defined in equation (50), the integration yields

$$\begin{aligned} \langle k_2 | T_0 | k_1 \rangle &= -\frac{\eta k}{2k_1 k_2} \left[D\left(\frac{\rho - 1}{\rho + 1}\right) - D\left(\frac{\rho + 1}{\rho - 1}\right) \right] \Bigg|_{\mu=-1}^{\mu=+1} \\ &= \frac{\eta k}{2k_1 k_2} \left[D(uv) + D\left(\frac{1}{uv}\right) - D\left(\frac{u}{v}\right) - D\left(\frac{v}{u}\right) \right] \end{aligned} \tag{96}$$

This equation is identical to equation (62), which gives the result for $\langle k_2 | T_0 | k_1 \rangle$ in the shielded case when only the R-independent terms are included, that is, the result for $\langle k_2 | T_0^{(\infty)} | k_1 \rangle$. Although it is beyond the scope of this report to examine in detail the exact form of $T_\ell^{(\infty)}$ for $\ell > 0$, the evidence presented here leaves little reason to doubt the equivalence of $T^{(\infty)}$ and Hostler's formula.

CONCLUDING REMARKS

The Coulomb T matrix T(k) is obtained from the T matrix $T^{(R)}(k)$ for a screened Coulomb potential by the prescription

$$T^{(R)}(k) \to T(k) + \mathcal{O}\left(\frac{1}{R}\right) \qquad (R \to \infty)$$

Generally, it makes no difference whether k approaches the real axis before or after the limit $R \to \infty$ is taken, and in this general case

$$\langle \vec{k}_2 | T | \vec{k}_1 \rangle = \langle \vec{k}_2 | T^{(\infty)} | \vec{k}_1 \rangle = \frac{V_0}{2\pi^2} \frac{1 + M}{(\vec{k}_2 - \vec{k}_1)^2}$$

where M is given by Hostler's integral (5).

When $k = \pm|\vec{k}_1|$ or $k \to \pm|\vec{k}_2|$, however, the magnitude and phase of this equation are incorrect. Here it is important that k be allowed to approach the real axis before the limit $R \to \infty$. The result for $k \to \pm|\vec{k}_1|$ is

$$\langle \vec{k}_2 | T^{(R)} | \vec{k} \rangle \to \frac{e^{i\delta_0 - 2\pi\eta}}{C_0(\eta)} u^{i\eta} \langle \vec{k}_2 | T^{(\infty)} | \vec{k}_1 \rangle$$

$$= \frac{V_0}{2\pi^2} C_0(\eta) e^{i\delta_0} \frac{(k_2^2 - k^2)^{i\eta}}{\left[(\vec{k}_2 - \vec{k}_1)^2\right]^{1+i\eta}} + \mathcal{O}[(k \pm k_1)R] + \mathcal{O}\left(\frac{1}{R}\right)$$

The symmetry of $\langle \vec{k}_2 | T | \vec{k}_1 \rangle$ may be invoked to obtain the result for $k \to \pm|\vec{k}_2|$.

The Coulomb T matrix is seen to be independent of screening effects except when $k \to \pm|\vec{k}_1|$ or $k \to \pm|\vec{k}_2|$; at these points it depends directly on R only through the logarithmic phase factor $e^{i\delta_0}$. The magnitude of the T matrix becomes discontinuous in the limit of zero screening: for example, if k is on the real axis in the vicinity of k_1,

$$|\langle \vec{k}_2 | T | \vec{k}_1 \rangle| = \frac{V_0}{2\pi^2} \frac{1}{(\vec{k}_2 - \vec{k}_1)^2} \mathcal{M}_1 \mathcal{M}_2$$

where

$$\mathscr{M}_1 = \begin{cases} C_0(\eta) & \begin{cases} k_1 > k \\ k_1 = k \\ k_1 < k \end{cases} \\ 1 & \\ e^{\pi\eta} C_0(\eta) & \end{cases}$$

$$\mathscr{M}_1 = \begin{cases} C_0(\eta) & k_1 > k \\ 1 & k_1 = k \\ e^{\pi\eta} C_0(\eta) & k_1 < k \end{cases}$$

$$\mathscr{M}_2 = \begin{cases} C_0(\eta) & k_2 > k_1 \\ e^{\pi\eta} C_0(\eta) & k_2 < k_1 \end{cases}$$

Lewis Research Center,
National Aeronautics and Space Administration,
Cleveland, Ohio, February 5, 1965.

APPENDIX - ORDER OF MAGNITUDE ESTIMATE

In the investigation of $J_{\ell}(12)$, the quantity

$$\mathscr{F} = \int_R^\infty \omega_1(r) \int_r^\infty \omega_2(r') \, dr' \, dr$$

was neglected on the grounds that it could be shown to be of order $1/R$ unless both $k_2 \to k_1^2$ and $k^2 \to k_2^2$. Essentially the same integral was neglected in the detailed study of J_0 for the same reason. In this appendix, a rigorous estimate of the magnitude of $\mathscr{F}$ will be given.

If R is large enough, asymptotic forms may be used for ω_1 and ω_2, and $\mathscr{F}$ can be written as the sum of eight integrals all of the general form

$$P = \int_R^\infty \frac{e^{-\lambda r}}{r^{1+\alpha}} \int_r^\infty \frac{e^{-\mu s}}{s^{1+\beta}} \, ds \, dr \tag{A1}$$

The various values of λ and μ will be $\pm ik_2 \pm ik$ and $\pm ik_1 - ik$, respectively, and thus they satisfy the conditions

$$\left.\begin{aligned} \mathscr{R}e(\mu) &> 0 \\ \mathscr{R}e(\mu + \lambda) &\geq 0 \end{aligned}\right\} \tag{A2}$$

It is convenient to write P in the form

$$P = \int_R^\infty \frac{g(r)}{r^{1+\alpha}} \, dr \tag{A3}$$

where

$$g(r) \equiv e^{-\lambda r} \int_r^\infty \frac{e^{-\mu s}}{s^{1+\beta}} \, ds = \frac{e^{-(\mu+\lambda) r}}{r^\beta} \Psi(1, 1 - \beta; \mu r) \tag{A4}$$

$$g(r) = \frac{e^{-(\mu+\lambda) r}}{\beta r^\beta} \left[\Phi(1, 1 - \beta; \mu r) - \Gamma(1 - \beta)(\mu r)^\beta e^{\mu r}\right] \tag{A5}$$

Equation (A4) may be used to show that

$$h(r) \equiv \mu r g(r) \tag{A6}$$

is bounded as $r \to \infty$ if μ is fixed; and equation (A5) may be used to show that $g(r)$ is bounded for all $r \geq R$ even if $\mu \to 0$. Thus, if μ is fixed,

$$P = \frac{1}{\mu} \int_R^\infty \frac{h(r)}{r^{2+\alpha}}\, dr = \mathcal{O}\left(\frac{1}{\mu R}\right) \qquad \text{as} \begin{cases} R \to \infty \\ \mu R \to \infty \end{cases} \tag{A7}$$

(Note that this result is independent of the value of λ.) If $\mu \to 0$, however, it is necessary to integrate equation (A1) once by parts and write

$$P = \frac{g(R)}{\lambda R^{1+\alpha}} - \frac{1}{\lambda} \int_R^\infty \left[\frac{e^{-(\lambda+\mu)r}}{r^\beta} + (1 + \alpha) g(r)\right] \frac{dr}{r^{2+\alpha}} \tag{A8}$$

Now, since $g(r)$ is bounded even for $\mu \to 0$, the integral is of order $1/R$ and

$$P = \mathcal{O}\left(\frac{1}{\lambda R}\right) \qquad \text{as} \begin{cases} R \to \infty \\ \mu R \to 0 \end{cases} \tag{A9}$$

Equations (A7) and (A9) together show that P is of order $1/R$ unless both λ and μ approach zero.

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