

Coulomb T matrix “half-off-shell” at zero momentum, and for large l

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Recently Talukdar *et al.* [Phys. Rev. A **29**, 1865 (1984)] found that the so-called “half-off-shell” Coulomb T matrix $t_{Cl}(p, k; k^2)$ were to be (i) singular at $p = 0$ for $l > 0$, and (ii) increasing for increasing l . We point out that both these results are incorrect: (i) From the simple closed formula

$$t_{Cl}(p, k; k^2) = (2\gamma/\pi p) \exp(3\pi\gamma/2) Q_l^\gamma[(p^2 + k^2)/2pk], \quad 0 < p < k,$$

one can see by inspection that $t_{Cl}(p, k; k^2) = O(p^l)$, for $p \rightarrow 0$, precisely as the Coulomb-potential matrix element and the off-shell Coulomb T matrix. (γ is Sommerfeld’s parameter and Q_l^γ is Legendre’s function of the second kind.) (ii) For all $p \neq k$, $t_{Cl}(p, k; k^2)$ tends exponentially to zero as l tends to infinity: as $l^{-1/2} \exp[-l|\ln(p/k)|]$.

The partial-wave- (PW) projected “half-off-shell” T matrix associated with the Coulomb potential $V_{Cl}(r) = 2k\gamma/r$ (γ is Sommerfeld’s parameter, $k\gamma$ is a real constant) can be defined by¹

$$t_{Cl}(p, k; k^2) = \langle p | V_{Cl} | kl + \rangle_C, \quad \text{for } p \neq k, \quad (1)$$

where $|kl + \rangle_C$ is the PW Coulomb scattering state at energy $k^2 > 0$ ($\text{Im}k \neq 0$, units are such that $\hbar = 1 = 2m$), and p is the off-shell ($p \neq k$) momentum. A convenient closed expression for $\langle p | V_{Cl} | kl + \rangle_C$ is most easily obtained by PW projection of the full “half-off-shell” Coulomb T matrix, which equals^{1,2}

$$\langle p | V_C | \mathbf{k} + \rangle_C = k\gamma\pi^{-2}\Gamma(1+i\gamma)e^{-\pi\gamma/2} \lim_{\epsilon \rightarrow 0} [p^2 - (k+i\epsilon)^2]^{i\gamma} (|\mathbf{p} - \mathbf{k}|^2 + \epsilon^2)^{-1-i\gamma}, \quad (2)$$

where $|\mathbf{k} + \rangle_C$ is the full Coulomb scattering state at positive energy k^2 . By using³

$$\Gamma(1+\mu) \int_{-1}^1 P_l(x)(z-x)^{-\mu-1} dx = 2(z^2-1)^{-\mu/2} e^{-i\pi\mu} Q_l^\mu(z), \quad |\arg(z-1)| < \pi, \quad l=0, 1, \dots, \quad (3)$$

where Q_l^μ is Legendre’s function of the second kind, one easily obtains^{4,5}

$$\langle p | V_{Cl} | kl + \rangle_C = 2\gamma(\pi p)^{-1} e^{\pi\gamma/2} Q_l^\gamma(u) \delta, \quad \text{for } p \neq k, \quad (4)$$

where $u := (p^2 + k^2)/(2pk)$ and^{6,7}

$$\delta := \begin{cases} e^{\pi\gamma} & \text{if } 0 < p < k, \\ 1 & \text{if } 0 < k < p. \end{cases} \quad (5)$$

$$\langle p | V_{Cl} | kl + \rangle_C = i(\pi p)^{-1} e^{-\pi\gamma/2} l! \frac{\Gamma(1+i\gamma)\Gamma(1-i\gamma)}{\Gamma(l+1-i\gamma)} \lim_{\epsilon \rightarrow 0} [a^{i\gamma} P_l^{(i\gamma, -i\gamma)}(u) - (a^*)^{-i\gamma} P_l^{(-i\gamma, i\gamma)}(u)], \quad \text{for } p \neq k, \quad (8)$$

where

$$a := (p - k - i\epsilon)/(p + k + i\epsilon),$$

and $P_l^{(\dots)}$ is Jacobi’s polynomial of degree l . One easily verifies that Eqs. (4) and (8) are equivalent.⁴ From Eq. (8) we see clearly that

$$\Gamma(l+1-i\gamma) \langle p | V_{Cl} | kl + \rangle_C$$

is real for real p , k , and γ ; it follows directly from known

In view of the well-known relation

$$\lim_{z \rightarrow \infty} [z^{l+1} Q_l^\mu(z)] = e^{i\pi\mu} \frac{\Gamma(l+1+\mu)}{(2l+1)!!}, \quad (6)$$

one has

$$\lim_{p \rightarrow 0} [p^{-l} \langle p | V_{Cl} | kl + \rangle_C] = k\gamma\pi^{-1} (2/k)^{l+2} e^{\pi\gamma/2} \frac{\Gamma(l+1+i\gamma)}{(2l+1)!!}, \quad (7)$$

which shows that the PW Coulomb “half-off-shell” T matrix is of the order p^l for $p \rightarrow 0$.

Another convenient closed form for $\langle p | V_{Cl} | kl + \rangle_C$ is^{4,8}

properties of $|kl + \rangle_C$ that it has to be real. Notice that

$$\text{Im} \langle p | V_{Cl} | kl + \rangle_C / \text{Re} \langle p | V_{Cl} | kl + \rangle_C = \tan \sigma_l(k), \quad (9)$$

where $\sigma_l(k)$ is the Coulomb phase shift.

Let us denote the equation obtained from Eq. (8) upon replacing both Jacobi polynomials through use of the equality

$$P_l^{(\alpha, -\alpha)}(u) = \begin{Bmatrix} l+\alpha \\ l \end{Bmatrix} {}_2F_1(-l, l+1; 1+\alpha; (1-u)/2) \quad (10)$$

by Eq. (8)'. As far as we know, Eq. (8)' in its essential form was published for the first time by Dolinskii and Mukhamedzhanov.⁸

I. BEHAVIOR AT $p = 0$

Recently Maximon,⁹ and subsequently Talukdar, Ghosh, and Sasakawa¹⁰ derived once more essentially Eq. (8)' (transliteration: $p \rightarrow q$ and $\gamma \rightarrow \eta$); however, in Eq. (17) of Ref. 10 the limit for $\epsilon \rightarrow 0$ has been carried out in an ambiguous way, viz., when $0 < p < k$.

It is claimed in Ref. 10 that $t_{Cl}(p, k; k^2)$ for $l > 0$ were to be singular at $p = 0$, and in Sec. III numerical results supporting this claim are reported; see Figs. 1-4 of Ref. 10. Unfortunately this claim is at variance with Eqs. (4) and (7), and consequently these numerical data must be considered incorrect.

It is noteworthy that either term inside the square brackets on the right-hand side of Eq. (8) is $O(p^{-l})$ for $p \rightarrow 0$, and hence (highly) singular if $l > 0$. Apparently, the proper combination of these two terms effectuates that the pole of order l cancels, even in such a delicate way that a zero of order $l + 1$ results, at $p = 0$.

This important observation leads us to suggesting two possible sources of computational error in the numerical evaluation of the Coulomb half-shell T matrix for small momenta:

(A) The limit for $\epsilon \downarrow 0$ in Eq. (8)' is incorrectly evaluated in the case $0 < p < k$. Note that [cf. Eq. (5)]

$$\lim_{\epsilon \downarrow 0} a^{i\gamma} = \begin{cases} e^{+\pi\gamma} |(k-p)/(k+p)|^{i\gamma}, & \text{if } 0 < p < k, \\ |(k-p)/(k+p)|^{i\gamma}, & \text{if } 0 < k < p, \end{cases} \quad (11)$$

whereas

$$\lim_{\epsilon \downarrow 0} (a^*)^{i\gamma} = \begin{cases} e^{-\pi\gamma} |(k-p)/(k+p)|^{i\gamma}, & \text{if } 0 < p < k, \\ |(k-p)/(k+p)|^{i\gamma}, & \text{if } 0 < k < p. \end{cases} \quad (12)$$

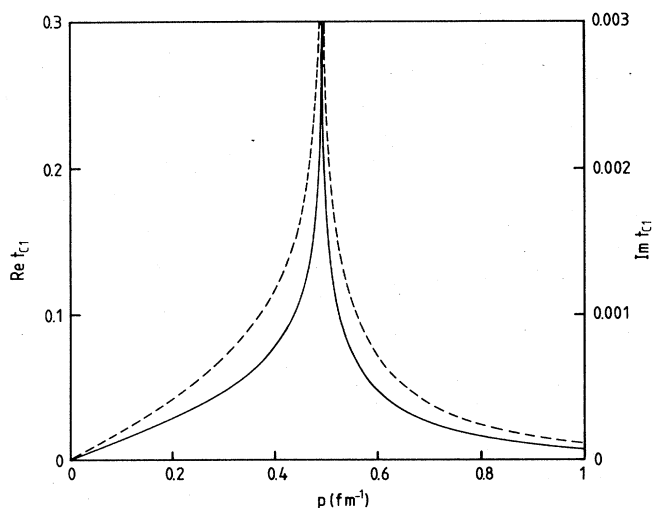


FIG. 1. The quantity $t_{Cl}(p, k; k^2) := \langle p | V_{Cl} | kl + \rangle_C$ for $l = 1$, as a function of p . Same parameters as in Ref. 10, Figs. 1-4, bottom. Solid and dashed lines represent the real and imaginary parts, respectively, of t_{Cl} . The singular behavior near $p = k \approx 0.5 \text{ fm}^{-1}$ cannot be clearly seen on the scale of the figure.

Obviously, if these factors $e^{\pm\pi\gamma}$ are not correctly taken into account, the pole of order l at $p = 0$ in either term involving the Jacobi polynomial does not cancel, so that in the final expression for t_{Cl} , a pole of order $l + 1$ at $p = 0$ will be found.

(B) There is numerical inaccuracy due to the delicacy of the way in which the two terms inside the square brackets in Eqs. (8) or (8)', each having a pole of order l , taken together produce a zero of order $l + 1$.

Source (A) must have been appreciated by the authors of Ref. 10, because Ref. 9 gives a careful analysis of this point. Therefore, we believe that source (B) is the reason for the false claim made in Ref. 10 on the behavior of $t_{Cl}(p, k; k^2)$ for $l > 0$ at $p = 0$.

II. BEHAVIOR FOR $l \rightarrow \infty$

In Figs. 5 and 6 of Ref. 10 and the covering text, it is reported that the real and imaginary parts of $t_{Cl}(p, k; k^2)$ were to be increasing for increasing l , in a certain case even exponentially (although stated above Fig. 5 is "diverges loga-

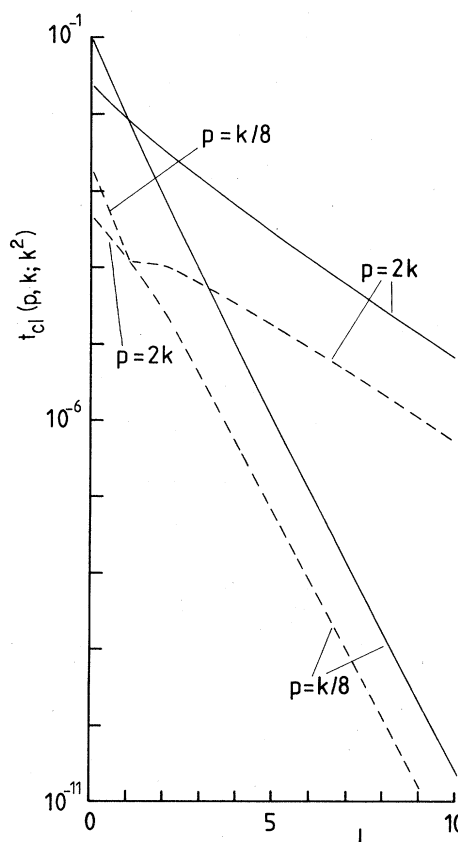


FIG. 2. The quantity $t_{Cl}(p, k; k^2)$ for $p = k/8$ and for $p = 2k$, as a function of $l: l = 0, 1, 2, \dots$. The solid line connects the results for the real parts, which are positive for all l . The dashed line connects the results for the imaginary parts, which are positive for $l = 1, 2, \dots, 10$. For $l = 0$ $\text{Im} t_{Cl}$ is negative in both cases, and we have plotted $|\text{Im} t_{Cl}|$. This is the reason for the apparent discontinuity in the slope of these lines at $l = 1$. This apparent discontinuity is of no significance: Each line merely serves to guide the eye, and to connect the eleven points for $l = 0, 1, \dots, 10$.

rithmically").

Again, this must be considered incorrect, as we shall briefly show. From Ref. 11, p. 136, Eq. (44) or Ref. 12, p. 162, Eq. (31) we get

$$Q_\nu^\mu(u) = e^{i\pi\mu}(\pi pk)^{1/2}|p^2 - k^2|^{-1/2} \exp[-(\nu + \frac{1}{2})|\ln(p/k)|] \nu^{\mu-1/2}[1 + O(\nu^{-1})], \quad \text{as } \nu \rightarrow \infty, \quad (13)$$

where $p \neq k$ and $u := (p^2 + k^2)/2pk$ as before. Thus we obtain from Eq. (4), for $l \rightarrow \infty$:

$$\langle p | V_{Cl} | kl + \rangle_C = \begin{cases} 2\gamma\pi^{-1/2}e^{\pi\gamma/2}(k^2 - p^2)^{-1/2}(p/k)^{l+\gamma-1/2}[1 + O(l^{-1})], & \text{if } 0 < p < k, \\ 2\gamma\pi^{-1/2}e^{-\pi\gamma/2}(p^2 - k^2)^{-1/2}(k/p)^{l+1+\gamma-1/2}[1 + O(l^{-1})], & \text{if } 0 < k < p. \end{cases} \quad (14)$$

Obviously $\langle p | V_{Cl} | kl + \rangle_C$ tends exponentially to zero as l tends to infinity, for all $p \neq k$, as $l^{-1/2} \exp(-l|\ln(p/k)|)$.

It is interesting to note that either term inside the square brackets on the right-hand side of Eq. (8) is exponentially increasing in l , for $l \rightarrow \infty$. By using Ref. 11, p. 142, Eq. (21) or Ref. 12, p. 154, we obtain

$$\left| \frac{p-k}{p+k} \right|^{l\gamma} P_l^{(i\gamma, -i\gamma)} \left(\frac{p^2+k^2}{2pk} \right) = (pk/\pi)^{1/2}|k^2 - p^2|^{-1/2} \exp[(l + \frac{1}{2})|\ln(p/k)|] l^{-1/2}[1 + O(l^{-1})], \quad \text{as } l \rightarrow \infty, \quad \text{for } p \neq k, \quad (15)$$

which clearly tends to infinity as $l^{-1/2} \exp(+l|\ln(p/k)|)$. Apparently, the proper combination of these two terms in Eq. (8) effectuates that the exponentially increasing behavior disappears, even in such a manner that an exponentially decreasing (to zero) behavior results, for $l \rightarrow \infty$. In analogy with our previous remark, we suggest that this delicate combination of two "singular" (at $l = \infty$) terms resulting in a "very regular" term may be the "explanation" of the incorrect results reported in Ref. 10.

In this connection, it is interesting to note that the PW series for $\langle p | V_C | k + \rangle_C$, which reduces essentially to

$$\sum_{l=0}^{\infty} (2l+1) P_l(\hat{p} \cdot \hat{k}) Q_l^\nu(u), \quad (16)$$

is convergent ($|k + \rangle_C$ is the full Coulomb scattering state).

More general series of products of Legendre functions have been evaluated in Ref. 13; conditions for the convergence of such series follow easily from Eqs. (13) and (15).

For the behavior of the off-shell Coulomb T matrix $\langle p | T_{Cl} | p' \rangle$ at $p=0$, $p=k$, $p'=k$, $p=\infty$, and $l=\infty$, the reader is referred to Refs. 14 and 15.

Finally, for comparison with the numerical results reported in Ref. 10, we show in Fig. 1 the p wave ($l=1$) $t_{Cl}(p, k; k^2)$ as a function of p , for parameter values corresponding to the bottom case of Fig. 2 of Ref. 10. The regular (linear) behavior near $p=0$ is clearly seen. Further, in Fig. 2 we show for the same parameter values $t_{Cl}(p, k; k^2)$ for increasing l , for $p=k/8$, and $p=2k$, respectively. The correct decreasing exponential behavior, $\propto l^{-1/2} \times \exp(-l|\ln(p/k)|)$, is clearly illustrated. Note that the same case has been depicted incorrectly in Fig. 6 of Ref. 10.

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