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Off-Shell and On-Shell Unitarity Relations in Two-Body Coulomb Scattering*

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It is demonstrated that the Coulomb T matrix $T(\vec{p}_2, \vec{p}_1; E \pm i\eta)$ satisfies a modified off-shell unitarity relation with a phase factor which depends upon the region from which the on-shell limit is approached. However, the on-shell Coulomb unitarity relation is not well defined. The discontinuities across the on-shell Coulomb cut in the p_2 and p_1 planes are evaluated.

Recently, there has been an increasing interest in the unitarity relation for two-body Coulomb scattering. This interest is motivated partly from recent attempts at applying the Fadeev equations to three-body atomic collisions.[1-5] From the work of Nuttall and Stagat,[6] it is clear that the Coulomb T matrix $T(\vec{p}_2, \vec{p}_1; E)$ satisfies a modified off-shell unitarity relation and that its discontinuity across the unitarity cut is not zero. The off-shell Coulomb unitarity relation of Nuttall and Stagat, which is evaluated only for the $p_2 < k$ and $p_1 < k$ ($k^2 = 2\mu E$) region, can be easily generalized to other regions. The purpose of the present communication is to show that due to the on-shell Coulomb cut the off-shell Coulomb unitarity relation does not have a well-defined on-shell limit. The discontinuities across the on-shell Coulomb cut in the p_2 and p_1 planes are evaluated.

A mathematically well-defined integral representation of the two-body off-shell Coulomb T matrix has been derived by Schwinger,[7]

$$T(\vec{p}_2, \vec{p}_1; E) = \frac{1}{2\pi^2} \frac{Ze^2}{|\vec{p}_2 - \vec{p}_1|^2} \times \left(1 - \frac{4i\nu}{e^{2\pi\nu} - 1} \int_{C_0} \frac{dt\, t^{-i\nu}}{\epsilon(1-t)^2 - 4t}\right), \quad (1)$$

with

$$\nu = -Ze^2(\mu/2E)^{1/2}, \quad (2)$$

$$\epsilon = \frac{(k^2 - p_2^2)(k^2 - p_1^2)}{k^2 |\vec{p}_2 - \vec{p}_1|^2}. \quad (3)$$

This can be evaluated to give[5,8]

$$T(\vec{p}_2, \vec{p}_1; E) = \frac{1}{2\pi^2} \frac{Ze^2}{|\vec{p}_2 - \vec{p}_1|^2} (\tau_a + \tau_b), \quad (4)$$

with

$$\tau_a = 1 - \frac{1}{(1+\epsilon)^{1/2}} \left(1 + \sum_{n=1}^{\infty} \frac{2\nu^2}{n^2 + \nu^2} t_+^n\right), \quad (5)$$

$$\tau_b = \frac{2\pi\nu}{e^{2\pi\nu} - 1} \left(\frac{t_+^{-i\nu}}{(1+\epsilon)^{1/2}}\right), \quad (6)$$

$$t_\pm \equiv (1 + 2/\epsilon) \mp (2/\epsilon)(1+\epsilon)^{1/2}, \quad (7)$$

where μ is the reduced mass and Z is the product of the charges of the two particles.

Due to the long-range effect, the off-shell Coulomb T matrix does not approach a well-defined limit as $p_2 \to k$ or $p_1 \to k$ on the energy shell.[7-9] Thus for the $E > 0$ case, it is necessary to examine the different regions from which the on-shell limit may be approached.[9] There are four such regions:

$$\begin{aligned} &\text{region I:} && p_2 > k \text{ and } p_1 > k, \\ &\text{region II:} && p_2 > k > p_1, \\ &\text{region III:} && p_2 < k \text{ and } p_1 < k, \\ &\text{region IV:} && p_2 < k < p_1. \end{aligned} \quad (8)$$

For the case where E is replaced by $E + i\eta$, it can be shown that the quantity t_+ in these four regions takes on the following different forms in the limit of $\eta \to 0^+$:

$$t_+ = |t_+| \exp\begin{cases} 2i\pi & \text{for region I} \\ i\pi & \text{for regions II and IV} \\ 0 & \text{for region III}. \end{cases} \quad (9)$$

These phase relations must be explicitly considered in examining the unitarity relations. The off-shell unitarity relation may be written as

$$T(\vec{p}_2, \vec{p}_1; E + i\eta) - T(\vec{p}_2, \vec{p}_1; E - i\eta)$$
$$= \int d\vec{p}'\, T(\vec{p}_2, \vec{p}'; E + i\eta)[(E - p'^2/2\mu + i\eta)^{-1}$$

$$-(E-p'^2/2\mu-i\eta)^{-1}]T(\vec{p}',\vec{p}_1;E-i\eta)\ . \quad (10)$$

The left-hand side (lhs) of the unitarity relation

$$(T-T^\dagger)^{\text{lhs}}=T(\vec{p}_2,\vec{p}_1;E+i\eta)-T(\vec{p}_2,\vec{p}_1;E-i\eta) \quad (11)$$

is just the discontinuity of τ_b across the unitarity cut

$$(T-T^\dagger)^{\text{lhs}}=\frac{Ze^2}{\pi|\vec{p}_2-\vec{p}_1|^2}\left(\frac{4\nu}{e^{2\pi\nu}-1}\right)\times\left(\frac{e^{2\pi\nu}[t_+^*]^{i\nu}}{[t_+^*-t_-^*]\epsilon^*}-\frac{[t_+]^{-i\nu}}{(t_+-t_-)\epsilon}\right)\ . \quad (12)$$

The phase relation between t_+ and t_+^* can be expressed as

$$\arg[t_+^*]=2\pi-\arg[t_+]\ . \quad (13)$$

Then Eq. (12) may be rewritten as

$$(T-T^\dagger)^{\text{lhs}}=\frac{Ze^2}{\pi|\vec{p}_2-\vec{p}_1|^2}\left(\frac{4\nu/\epsilon}{e^{2\pi\nu}-1}\right)\times\left(\frac{|t_+|^{i\nu}-|t_-|^{i\nu}}{t_+-t_-}\right)e^{\nu\arg[t_+]}\ , \quad (14)$$

where $\arg[t_+]$ is given by Eq. (9) in the limit of $\eta\to 0^+$.

Since the contribution to the integral on the right-hand side (rhs) of the unitarity relation comes primarily from values of $p_1'=k$, where $\epsilon=0$, the τ_a part of T, which may be expanded in powers of ϵ,

$$\tau_a=\frac{\epsilon}{2(1+\nu^2)}-\frac{3\epsilon^2}{2(4+\nu^2)(1+\nu^2)}+O(\epsilon^3) \quad (15)$$

does not contribute to the right-hand side of the unitarity relation. We have therefore

$$(T-T^\dagger)^{\text{rhs}}=\frac{Z^2e^4}{4\pi^4}\int d\vec{p}'\,\frac{\tau_b}{|\vec{p}_2-\vec{p}'|^2}\times\left[\left(E-\frac{p'^2}{2\mu}+i\eta\right)^{-1}-\left(E-\frac{p'^2}{2\mu}-i\eta\right)^{-1}\right]\frac{\tau_b^\dagger}{|\vec{p}'-\vec{p}_1|^2} \quad (16a)$$

$$=\left(\frac{Ze^2\nu}{\pi}\right)^2\frac{2\mu e^{2\pi\nu}}{(e^{2\pi\nu}-1)^2}\times\left[\frac{(k^2-p_1^2-i\eta)(k^2+i\eta)}{(k^2-p_2^2+i\eta)(k^2-i\eta)}\right]^{i\nu}I(k)J(k)\ , \quad (16b)$$

with

$$I(k)=\int_0^\infty dp'\,p'^2\left(\frac{k^2-p'^2-i\eta}{k^2-p'^2+i\eta}\right)^{i\nu}\times\left(\frac{1}{k^2-p'^2+i\eta}-\frac{1}{k^2-p'^2-i\eta}\right) \quad (17)$$

and

$$J(k)=\int\frac{d\hat{k}}{|\vec{p}_2-\vec{k}|^2|\vec{k}-\vec{p}_1|^2}\left(\frac{|\vec{p}_2-\vec{k}|^2}{|\vec{k}-\vec{p}_1|^2}\right)^{i\nu}\ , \quad (18)$$

where in Eq. (16b) we have made use of the $p'=k$ peaking approximation.

The integral $I(k)$ over the singular terms has been evaluated by Nuttall and Stagat[6]:

$$I(k)=-ik\,e^{-2\pi\nu}\int_{\tan^{-1}(\eta/k^2)}^{\tan^{-1}(\eta/\infty)}e^{2\nu\theta}d\theta$$

$$\underset{\eta\to 0^+}{=}\ -i\pi k\,e^{-2\pi\nu}\left(\frac{e^{2\pi\nu}-1}{2\pi\nu}\right)\ . \quad (19)$$

The integral $J(k)$ given by Eq. (18) does not involve the $\eta\to 0^+$ limit. It has been evaluated by Nuttall and Stagat for the off-shell case,[6]

$$J(k)=\frac{i\pi}{|\vec{p}_2-\vec{p}_1|^2}\left(\frac{4\nu/\epsilon}{z^2e^4\mu^2}\right)\left(\frac{k^2-p_2^2}{k^2-p_1^2}\right)^{i\nu}\times\frac{|t_+|^{i\nu}-|t_-|^{i\nu}}{t_+-t_-}\ . \quad (20)$$

On the energy shell, $J(k)$ given by Eq. (18) may be rewritten as

$$J(k)=[(2\mu Ze^2)^{-2}\int d\hat{k}f(\hat{p}_2\cdot\hat{k})f^*(\hat{k}\cdot\hat{p}_1]_{p_2=p_1=k}\ , \quad (21)$$

with

$$f(\hat{p}_i\cdot\hat{k})=-\frac{2\mu z e^2}{|\vec{p}_i-\vec{k}|^2}\left(\frac{4k^2}{|\vec{p}_i-\vec{k}|^2}\right)^{-i\nu}e^{2i\arg[\Gamma(1-i\nu)]}\ , \quad (22)$$

where $f(\hat{p}_i\cdot\hat{k})$ is the Coulomb scattering amplitude. Thus, on the energy shell, the integral yields[10]

$$J(k)=(4\pi/k)(2\mu Ze^2)^{-2}\,\mathrm{Im}f(\hat{p}_2\cdot\hat{p}_1)\ . \quad (23)$$

The right-hand side of the off-shell unitary relation can now be immediately obtained from Eqs. (16b), (19), and (20) by taking the $\eta\to 0^+$ limit. With the help of the relation

$$\lim_{\eta\to 0^+}\left(\frac{(k^2-p_1^2-i\eta)(k^2+i\eta)}{(k^2-p_2^2+i\eta)(k^2-i\eta)}\right)=\left(\frac{k^2-p_1^2}{k^2-p_2^2}\right)e^{-i\arg[t_+]}\ , \quad (24)$$

we obtain

$$(T-T^\dagger)^{\text{rhs}}=\frac{Ze^2}{\pi|\vec{p}_2-\vec{p}_1|}\left(\frac{4\nu/\epsilon}{e^{2\pi\nu}-1}\right)\times\left(\frac{|t_+|^{i\nu}-|t_-|^{i\nu}}{t_+-t_-}\right)e^{\nu\arg[t_+]}, \quad (25)$$

which is identical to $(T-T^\dagger)^{\text{lhs}}$ given by Eq. (14). This demonstrates that the Coulomb T matrix satisfies a modified off-shell unitarity relation. This result has been obtained previously by Nuttall and Stagat for region III [Eq. (8)] in which $\arg[t_+]=0$ in the $\eta\to 0^+$ limit.

On the energy shell, the limit of $\eta\to 0^+$ should be taken after setting $p_1 = k$ and $p_2 = k$. The right-hand side of the unitarity relation obtained from Eqs. (16b), (19), and (23) takes the form

$$(T - T^\dagger)^{\text{rhs}}_{p_1=p_2=k} = 2i\,\text{Im}\left[\frac{2\pi\nu e^{\pi\nu}}{e^{2\pi\nu}-1}\left(-\frac{1}{4\pi^2\mu}f(\hat{p}_2\cdot\hat{p}_1)\right)\right]. \tag{26}$$

The left-hand side of the on-shell unitarity relation can be obtained from Eq. (12). Near the energy shell, we have

$$t_+ \cong \tfrac{1}{4}\epsilon, \quad t_+^* \cong \tfrac{1}{4}\epsilon^*. \tag{27}$$

Equation (12) reduces to the form

$$(T - T^\dagger)^{\text{lhs}}_{p_1=p_2=k} = \frac{Ze^2}{\pi|\vec{p}_2-\vec{p}_1|^2}\,\frac{\nu}{e^{2\pi\nu}-1}\left[e^{2\pi\nu}\left(\frac{\epsilon^*}{4}\right)^{i\nu} - \left(\frac{\epsilon}{4}\right)^{i\nu}\right]$$

$$= 2i\,\text{Im}\{[g(k)]^2[-(1/4\pi^2\mu)f(\hat{p}_2\cdot\hat{p}_1)]\}, \tag{28}$$

with

$$g(k) = \lim_{p_i\to k} g(p_i) = \Gamma(1-i\nu)\,[4k^2]^{i\nu}e^{-i\nu\ln\eta} \tag{29}$$

and

$$g(p_i) = [(k^2 - p_i^2 + i\eta)/4k^2]^{-i\nu}\,\Gamma(1-i\nu)\,e^{-\pi\nu/2}. \tag{30}$$

The $g(p_i)$ are the Coulomb distortion factors.

From Eqs. (26) and (28), it is apparent that the on-shell unitarity is not well-defined for Coulomb scattering. This is a consequence of the fact that $T(\vec{p}_2, \vec{p}_1; E)$ does not approach a well-defined on-shell limit. We have on the energy shell

$$\lim_{p_1\to k} T(\vec{p}_2, \vec{p}_1; E + i\eta) = \lim_{p_1\to k}\{g(p_2)[-(1/4\pi^2\mu)f(\hat{p}_2\cdot\hat{p}_1)]g(p_1)\}. \tag{31}$$

It can be shown that $p_1 = k$ is actually a branch-point singularity in the T matrix. This gives rise to a branch cut on the initial half of the energy shell in the p_1 plane. The discontinuity across the on-shell Coulomb cut can be defined as

$$T - T^{\ddagger} \equiv T(\vec{p}_2, \hat{p}_1(p_1 + i\eta'); E) - T(\vec{p}_2, \hat{p}_1(p_1 - i\eta'); E), \tag{32}$$

with $\eta' \to 0^+$. Utilizing Eqs. (3)–(7) and Eq. (27), we find for the discontinuity

$$T - T^{\ddagger} = -\frac{1}{2\pi^2}\left(\frac{Ze^2}{|\vec{p}_2 - \vec{k}|^2}\right)\frac{4\pi\nu\sinh(\pi\nu/2)}{e^{2\pi\nu}-1} \times\left(\frac{2(k^2-p_2^2)}{k|\vec{p}_2-\vec{k}_2|^2}\right)^{-i\nu} e^{-i\nu\ln\eta'} \tag{33}$$

in the p_1 plane. The corresponding discontinuity across the Coulomb cut in the p_2 plane can be obtained from symmetry considerations upon replacing p_2 by p_1.

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