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Abstract. Analytic continuations into the left half of the complex angular momentum plane permit the derivation of some exact integral expressions for the attractive and repulsive Coulomb amplitudes. The problem of background integrals is thus removed and the expressions may be written either in a form which is suitable for expressing the amplitudes as a sum over all the Coulomb poles or as integrals in regions of the complex plane which contain no poles. The latter forms are extremely convenient for the application of the saddle-point method and are used to obtain the semiclassical limits for the amplitudes. All the terms of the Poisson summation formula are correctly taken into account and generalisations to other cases are discussed.

1. Integral representations for positive l

The amplitude for non-relativistic elastic scattering in a Coulomb potential $V(r)=z_1z_2e^2/r$ (where z_1e and z_2e are the target and projectile charges and r is their separation) is given (e.g. Landau and Lifshitz 1965) by

$$f(\theta)=\frac{-\eta}{2k\sin^2(\frac{1}{2}\theta)}\exp(2\mathrm{i}\sigma_0-2\mathrm{i}\eta\ln\sin(\tfrac{1}{2}\theta)). \tag{1}$$

In this equation $\sigma_0=\arg\Gamma(1+\mathrm{i}\eta)$, k is the wavenumber and the Sommerfeld parameter η is given by $\eta=z_1z_2e^2/\hbar v$, where v the relative velocity of the charges for large separations. Note that $\eta>0$ for a repulsive potential and $\eta<0$ for an attractive potential. The Rutherford cross section $\sigma_{\mathrm{R}}(\theta)=|f(\theta)|^2=\eta^2/[4k^2\sin^4(\frac{1}{2}\theta)]$ is independent of the sign of η though this is not true of the amplitude which satisfies $f(-\eta)=-f^*(\eta)$.

The partial wave representation of an elastic amplitude is usually written

$$f(\theta)=\frac{1}{2\mathrm{i}k}\sum_{l=0}^{\infty}(2l+1)P_l(\cos\theta)[S_l-1], \tag{2}$$

where $P_l(\cos\theta)$ are the Legendre polynomials and S_l are the elastic S-matrix elements. For Coulomb scattering

$$S_l=\Gamma(l+1+\mathrm{i}\eta)/\Gamma(l+1-\mathrm{i}\eta).$$

If the potential we are considering tends to zero sufficiently rapidly as $r\to\infty$ then the S-matrix elements tend to unity for large l (e.g. de Alfaro and Regge 1965) and the factor $[S_l-1]$ ensures convergence of the partial wave series. However, the infinite range of the Coulomb potential leads to a phase-shift ($\frac{1}{2}\arg S_l$) which is divergent for large l and the sum in equation (2) does not converge. It can, however, be shown (see

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the appendix) that this lack of convergence may simply be removed by writing the Coulomb amplitude of equation (1) as

$$f(\theta)=\frac{1}{2ik}\lim_{\alpha\to+0}\sum_{l=0}^{\infty}(2l+1)P_l(\cos\theta)S_l\exp[-\alpha(l+\tfrac{1}{2})^2], \tag{3a}$$

for $\theta\neq0$. The convergence factor has been chosen for our future convenience in § 3. We may now rewrite this amplitude using the integral transformations

$$f(\theta)=-\frac{1}{2k}\lim_{\alpha\to+0}\int_C\frac{\lambda P_{\lambda-\frac{1}{2}}(\cos\theta)}{\cos\pi\lambda}\exp[\pm i\pi(\lambda-\tfrac{1}{2})]S'_{\lambda-\frac{1}{2}}\,d\lambda \tag{3b}$$

and

$$f(\theta)=-\frac{1}{2k}\lim_{\alpha\to+0}\int_C\frac{\lambda P_{\lambda-\frac{1}{2}}(\cos(\pi-\theta))}{\cos\pi\lambda}S'_{\lambda-\frac{1}{2}}\,d\lambda, \tag{3c}$$

where $P_{\lambda-\frac{1}{2}}$ is the Legendre function of the first kind,

$$S'_{\lambda-\frac{1}{2}}=S_{\lambda-\frac{1}{2}}\exp(-\alpha\lambda^2)\qquad\text{with } S_{\lambda-\frac{1}{2}}=\Gamma(\lambda+\tfrac{1}{2}+i\eta)/\Gamma(\lambda+\tfrac{1}{2}-i\eta)$$

and C is any contour enclosing the positive real axis (but no poles of $S_{\lambda-\frac{1}{2}}$) in a clockwise direction and in a region of the complex plane where the integrals converge. (Throughout the paper λ is a continuous complex variable.) Equation (3c) is known as the Sommerfeld–Watson transformation and is obtained using

$$P_l(\cos(\pi-\theta))=(-1)^lP_l(\cos\theta)\qquad\text{for } l\geq0.$$

Equation (3b) may be used to obtain the Poisson summation formula by appropriately expanding $\cos\pi\lambda$ for λ just above and just below the real axis. We obtain

$$f(\theta)=\frac{1}{ik}\lim_{\alpha\to+0}\sum_{m=-\infty}^{\infty}(-1)^m\int_0^{\infty}\lambda P_{\lambda-\frac{1}{2}}(\cos\theta)S'_{\lambda-\frac{1}{2}}\exp(2\pi mi\lambda)\,d\lambda. \tag{4}$$

We may further split the amplitude by introducing the functions (Nussensweig 1965, Fuller 1975)

$$P^{\pm}_{\lambda-\frac{1}{2}}(\cos\theta)=\tfrac{1}{2}[P_{\lambda-\frac{1}{2}}(\cos\theta)\mp(2i/\pi)Q_{\lambda-\frac{1}{2}}(\cos\theta)], \tag{5}$$

where $Q_{\lambda-\frac{1}{2}}(\cos\theta)$ is the Legendre function of the second kind which has poles at $\lambda=-(l+\frac{1}{2})$, $l=0,1\ldots$, whose residues are just $P_l(\cos\theta)$ (Abramowitz and Stegun 1965). Using $P_{\lambda-\frac{1}{2}}=P^+_{\lambda-\frac{1}{2}}+P^-_{\lambda-\frac{1}{2}}$ we obtain

$$f(\theta)=\sum_{m=-\infty}^{\infty}(-1)^m(f^+_m+f^-_m), \tag{6}$$

with

$$f^{\pm}_m(\theta)=\frac{1}{ik}\lim_{\alpha\to+0}\int_0^{\infty}\lambda P^{\pm}_{\lambda-\frac{1}{2}}(\cos\theta)S'_{\lambda-\frac{1}{2}}\exp(2\pi mi\lambda)\,d\lambda. \tag{7a}$$

We see that for large λ the integrands in equation (7a) contain a factor $\exp(i\phi\lambda)$, with $\phi=2\pi m\pm\theta$. For $\phi\neq0$ (i.e. θ and m not both zero) it is possible to take each integral to infinity slightly above or below the real axis (e.g. along $\lambda=\mathrm{Re}\,\lambda(1\pm i\omega)$ with $0<\omega\ll1$) depending on whether $\phi\gtrless0$ and obtain an integral which is absolutely convergent without the factor $\exp(-\alpha\lambda^2)$. This factor then simply ensures that we pick up no additional contribution when we bring our integration path back on to the real axis at ∞. We may, therefore, drop the convergence factor completely (for $\theta \neq 0$) and write

$$f_m^{\pm}(\theta) = \frac{1}{ik}\int_0^{\infty} \lambda P_{\lambda-\frac{1}{2}}^{\pm}(\cos\theta) S_{\lambda-\frac{1}{2}} \exp(2\pi m i\lambda)\, d\lambda, \tag{7b}$$

where it is now implicit that the integrals are taken to ∞ in a region of the complex plane where they converge.

2. Usual derivation of the semiclassical limit

In the semiclassical limit the S-matrix may be written as $S_{\lambda-\frac{1}{2}} = \exp(2i\sigma(\lambda))$, where $\sigma(\lambda)$ is the WKB phase which is related to the classical deflection function $\Theta(\lambda)$ by $2\,\partial\sigma/\partial\lambda = \Theta(\lambda)$ (Newton 1966) with $\Theta(\lambda) = 2\tan^{-1}(\eta/\lambda)$ for the Coulomb potential. It is also usual to replace $P_{\lambda-\frac{1}{2}}^{\pm}(\cos\theta)$ by their asymptotic (large λ) approximations $\tilde{P}_{\lambda-\frac{1}{2}}^{\pm}$ (valid for $\lambda\sin\theta \gtrsim 1$)

$$P_{\lambda-\frac{1}{2}}^{\pm} \approx \tilde{P}_{\lambda-\frac{1}{2}}^{\pm} = \exp[\pm i(\lambda\theta - \tfrac{1}{4}\pi)]/(2\pi\lambda\sin\theta)^{1/2}. \tag{8}$$

The amplitudes $f_m^{\pm}$ now become

$$f_m^{\pm}(\theta) = \frac{1}{ik}\exp(\mp\tfrac{1}{4}i\pi)(2\pi\sin\theta)^{-1/2}\int_0^{\infty} \lambda^{1/2}\exp[i(\pm\lambda\theta + 2\sigma(\lambda) + 2\pi m\lambda)]\, d\lambda. \tag{9}$$

If we can find a real positive Λ which satisfies

$$\pm\theta + \Theta(\lambda) + 2\pi m = 0, \tag{10}$$

then, ignoring the variation of $\lambda^{1/2}$, the integrand of equation (9) has a point of stationary phase at the classical angular momentum Λ (i.e. the deflection function exists at an angle $\mp\theta - 2\pi m$ and there is a classical contribution to $f_m^{\pm}(\theta)$). Such terms may be evaluated by the method of stationary phase or the saddle-point method (Anni and Taffara 1974, Rowley and Marty 1976). All other terms are *assumed* to be negligible. For $\eta > 0$ the Coulomb deflection function lies between 0 and π for real positive λ and thus only the term $f_0^{-}(\theta)$ has a stationary point giving

$$f(\eta > 0) \approx f_0^{-}(\theta) = \frac{1}{ik}\int_0^{\infty} \lambda \tilde{P}_{\lambda-\frac{1}{2}}^{-}(\cos\theta) S_{\lambda-\frac{1}{2}}\, d\lambda. \tag{11a}$$

For $\eta < 0$ we have $-\pi < \Theta(\lambda) < 0$ for real positive λ and we obtain

$$f(\eta < 0) \approx f_0^{+}(\theta) = \frac{1}{ik}\int_0^{\infty} \lambda \tilde{P}_{\lambda-\frac{1}{2}}^{+}(\cos\theta) S_{\lambda-\frac{1}{2}}\, d\lambda. \tag{11b}$$

Note that since the lower limits of these integrals are zero the asymptotic expressions for $P_{\lambda-\frac{1}{2}}^{\pm}$ are not valid over some part of the integration paths. These limits are often replaced by $-\infty$ for analytic convenience.

The evaluation of the other terms $f_m^{\pm}(\theta)$ is very difficult for even if we close the integrals in the first or fourth quadrants of the complex λ-plane (so as to obtain no contribution at ∞) we are still left with unpleasant 'background' integrals along the imaginary axis. Therefore since equations (11*a*, *b*) (with the lower limits replaced by $-\infty$) do give the exact Coulomb amplitude in the semiclassical limit we shall examine this result in more detail. (Note that the semiclassical limit $\hbar \to 0$ is physically equivalent to $|\eta| \to \infty$).

We should note that for $\lambda \sin\theta \lesssim 1$ there are uniform approximations to $P_{\lambda-\frac{1}{2}}(\cos\theta)$ which are valid up to either $\theta = 0$ or $\theta = \pi$ (e.g. Berry 1969). We shall not, however, discuss these approximations since our main aim is to derive an *exact* integral expression for $f(\theta)$ which is valid for all $\theta \neq 0$, $\eta \neq 0$ and which correctly takes account of contributions from all values of m. We shall in fact show that for small $|\eta|$ the terms $m \neq 0$ contribute significantly to the cross section.

3. Negative λ

The analyticity of S in the left half-plane has been discussed by Singh (1962). For all λ (real or complex) we have the identities (Abramowitz and Stegun 1965)

$$S_{-\lambda-\frac{1}{2}} = S_{\lambda-\frac{1}{2}} \sin\pi(\lambda+\tfrac{1}{2}+\mathrm{i}\eta)/\sin\pi(\lambda+\tfrac{1}{2}-\mathrm{i}\eta) \tag{12}$$

and

$$P_{-\lambda-\frac{1}{2}}(\cos\theta) = P_{\lambda-\frac{1}{2}}(\cos\theta). \tag{13}$$

For integral values (i.e. $\lambda = l+\frac{1}{2}$) $P_{-l-1}(\cos\theta) = P_l(\cos\theta)$ and $S_{-l-1} = -S_l$ and since the convergence factor we have employed is invariant for $l \to -(l+1)$ we easily obtain

$$2f(\theta) = \frac{1}{2\mathrm{i}k} \lim_{\alpha\to+0} \sum_{l=-\infty}^{\infty} (2l+1)P_l(\cos\theta)S_l \exp[-\alpha(l+\tfrac{1}{2})^2], \tag{14}$$

where the summation now runs over both positive and *negative l*. We should note that although the Schrödinger equation defining $S_{\lambda-\frac{1}{2}}$ is invariant under $\lambda \to -\lambda$ this does not imply that the S-matrix is itself invariant under this transformation. Likewise no simple relationship between S_{-l-1} and S_l is guaranteed by the invariance of the equation for $l \to -(l+1)$. Indeed for an arbitrary potential the Schrödinger equation may not lead to a well defined S-matrix for $\mathrm{Re}\,\lambda < 0$ (de Alfaro and Regge 1965).

Equation (14) gives the integral transformations

$$2f(\theta) = -\frac{1}{2k} \lim_{\alpha\to+0} \int_\Gamma \frac{\lambda P_{\lambda-\frac{1}{2}}(\cos\theta)}{\cos\pi\lambda} \exp[\pm\mathrm{i}\pi(\lambda-\tfrac{1}{2})] S'_{\lambda-\frac{1}{2}}\, \mathrm{d}\lambda, \tag{15}$$

where Γ encloses the *entire* real axis. Note that the Sommerfeld–Watson form of the equation is no longer useful since $P_l(\cos(\pi-\theta)) = -(-1)^l P_l(\cos)$ for $l \leq -1$. Indeed

$$\lim_{\alpha\to+0} \int_\Gamma \frac{\lambda P_{\lambda-\frac{1}{2}}(\cos(\pi-\theta))}{\cos\pi\lambda} S'_{\lambda-\frac{1}{2}}\, \mathrm{d}\lambda = 0 \tag{16}$$

for the Coulomb S-matrix (see, however, § 6).

Using equation (15) we obtain the new Poisson summation formula

$$2f(\theta) = \frac{1}{\mathrm{i}k} \lim_{\alpha\to+0} \sum_{m=-\infty}^{\infty} (-1)^m \int_{-\infty}^{\infty} \lambda P_{\lambda-\frac{1}{2}}(\cos\theta) S'_{\lambda-\frac{1}{2}} \exp(2\pi m\mathrm{i}\lambda)\, \mathrm{d}\lambda. \tag{17}$$

Note that for $\eta > 0$ there are no poles of $S_{\lambda-\frac{1}{2}}$ in the upper half-plane. We may, therefore, take all the integrals with $m > 0$ to $\pm\infty$ slightly above the real axis (as in § 1) and drop the convergence factor. It is then only necessary to close these integrals in the upper half-plane to prove that they are all identically zero. The terms $m \leq 0$ are all non-zero due to the poles of $\Gamma(\lambda+\frac{1}{2}+i\eta)$ at $\lambda=-(l+\frac{1}{2}+i\eta)$. For $\eta<0$ it is the terms $m<0$ which identically vanish.

In equations (15) and (17) we may clearly use any function $\bar{S}_{\lambda-\frac{1}{2}}$ which reduces to S_l for $\lambda=l+\frac{1}{2}$. The problem is much simplified if we introduce

$$\bar{S}_{\lambda-\frac{1}{2}}=S_{\lambda-\frac{1}{2}}[1+\exp(-2\pi\eta)\exp(2\pi i\lambda)]/[1-\exp(-2\pi\eta)]. \tag{18}$$

This function has the properties $\bar{S}_l=S_l(l=0,\pm1,\dots)$ and

$$\bar{S}_{-\lambda-\frac{1}{2}}=\exp(-2\pi i\lambda)\bar{S}_{\lambda-\frac{1}{2}}. \tag{19}$$

Note also that all the poles of $S_{\lambda-\frac{1}{2}}$ have been suppressed though $\bar{S}_{\lambda-\frac{1}{2}}$ possesses an essential singularity at ∞.

Inserting $\bar{S}$ into equation (17) and using the usual technique for dropping the convergence factor we see that only the terms with $m=0$ and $m=-1$ are non-zero. Making the substitution $\lambda\to-\lambda$ we also see that these two terms are exactly equal giving

$$\begin{aligned} f(\theta)&=\frac{1}{ik}\lim_{\alpha\to+0}\int_{-\infty}^{\infty}\lambda P_{\lambda-\frac{1}{2}}(\cos\theta)\bar{S}'_{\lambda-\frac{1}{2}}\,d\lambda \\ &=-\frac{1}{ik}\lim_{\alpha\to+0}\int_{-\infty}^{\infty}\lambda P_{\lambda-\frac{1}{2}}(\cos\theta)\bar{S}'_{\lambda-\frac{1}{2}}\exp(-2\pi i\lambda)\,d\lambda. \end{aligned} \tag{20}$$

By using $P_{\lambda-\frac{1}{2}}=P^{+}_{\lambda-\frac{1}{2}}+P^{-}_{\lambda-\frac{1}{2}}$ we further obtain

$$\begin{aligned} f(\theta)&=\frac{1}{ik}\lim_{\alpha\to+0}\int_{-\infty}^{\infty}\lambda P^{-}_{\lambda-\frac{1}{2}+i\epsilon}(\cos\theta)\bar{S}'_{\lambda-\frac{1}{2}}\,d\lambda \\ &=-\frac{1}{ik}\lim_{\alpha\to+0}\int_{-\infty}^{\infty}\lambda P^{+}_{\lambda-\frac{1}{2}-i\epsilon}(\cos\theta)\bar{S}'_{\lambda-\frac{1}{2}}\exp(-2\pi i\lambda)\,d\lambda. \end{aligned} \tag{21}$$

The equality of these two formulae may be verified using the identity

$$P^{\pm}_{-\lambda-\frac{1}{2}}=P^{\mp}_{\lambda-\frac{1}{2}}\pm i\cot\pi(\lambda-\tfrac{1}{2})P_{\lambda-\frac{1}{2}}. \tag{22}$$

Both forms of equation (21) are valid irrespective of the sign of η. If we now take $\eta>0$ all the poles of $S_{\lambda-\frac{1}{2}}$ lie in the lower half-plane and the first form of equation (21) yields

$$f(\eta>0)=\frac{1}{ik[1-\exp(-2\pi\eta)]}\lim_{\alpha\to+0}\int_{-\infty}^{\infty}\lambda P^{-}_{\lambda-\frac{1}{2}+i\epsilon}(\cos\theta)S'_{\lambda-\frac{1}{2}}\,d\lambda. \tag{23a}$$

For $\eta<0$ the second form of equation (21) gives

$$f(\eta<0)=\frac{1}{ik[1-\exp(2\pi\eta)]}\lim_{\alpha\to+0}\int_{-\infty}^{\infty}\lambda P^{+}_{\lambda-\frac{1}{2}-i\epsilon}(\cos\theta)S'_{\lambda-\frac{1}{2}}\,d\lambda. \tag{23b}$$

Note the similarity between these *exact* expressions and their semiclassical counterparts equations (11*a*, *b*). Theses integrals are very convenient for the application of the saddle-point method. For example for $\eta>0$ the integration path may be deformed anywhere in the first, second and fourth quadrants without picking up any poles (subject to the condition that the integral must remain convergent). It is thus easy to follow the usual path which cuts the positive real axis at an angle of $-\frac{1}{4}\pi$ (Rowley and Marty 1976).

The other forms of equation (21) give integrals which are useful for expressing the amplitudes in terms of their respective poles. After a little manipulation we find for $\eta > 0$

$$f(\theta) = \frac{-1}{\mathrm{i}k[1+\exp(-2\pi\eta)]} \lim_{\alpha\to+0} \int_{-\infty}^{\infty} \lambda P^{+}_{\lambda-\frac{1}{2}-\mathrm{i}\epsilon}(\cos\theta) S'_{\lambda-\frac{1}{2}} \exp(-2\pi\mathrm{i}\lambda)\,\mathrm{d}\lambda \tag{24a}$$

and for $\eta < 0$

$$f(\theta) = \frac{-1}{\mathrm{i}k[1+\exp(2\pi\eta)]} \lim_{\alpha\to+0} \int_{-\infty}^{\infty} \lambda P^{-}_{\lambda-\frac{1}{2}+\mathrm{i}\epsilon}(\cos\theta) S'_{\lambda-\frac{1}{2}} \exp(2\pi\mathrm{i}\lambda)\,\mathrm{d}\lambda. \tag{24b}$$

4. Semiclassical limit

Using the reflection properties of $P_{\lambda-\frac{1}{2}}$ and $\bar{S}_{\lambda-\frac{1}{2}}$ we may use equations (20) to show that

$$f(\theta) = \frac{1}{\mathrm{i}k} \lim_{\alpha\to+0} \int_{0}^{\infty} \lambda P_{\lambda-\frac{1}{2}}(\cos\theta) S'_{\lambda-\frac{1}{2}} \left(1 - \frac{\exp(-2\pi\mathrm{i}\lambda)}{1-\exp(-2\pi\eta)} - \frac{\exp(2\pi\mathrm{i}\lambda)}{1-\exp(2\pi\eta)}\right) \mathrm{d}\lambda. \tag{25}$$

Comparing this with equation (4) we see that the integrals with $m \neq 0, \pm 1$ have been implicitly summed and give contributions which are just proportional to the $m = \pm 1$ terms. In the semiclassical limit the extra terms may clearly be neglected though they contribute significantly for small $|\eta|$. This result is not easily seen from a semiclassical argument since the terms never possess a stationary point. In the limit $|\eta| \to \infty$, equation (25) may be written

$$f(\theta) = \frac{1}{\mathrm{i}k} \lim_{\alpha\to+0} \int_{0}^{\infty} \lambda P_{\lambda-\frac{1}{2}}(\cos\theta) S'_{\lambda-\frac{1}{2}} [1 - \exp(\mp 2\pi\mathrm{i}\lambda)]\,\mathrm{d}\lambda \tag{26}$$

depending on whether $\eta \gtrless 0$. By introducing $P^{\pm}_{\lambda-\frac{1}{2}}$ the integrals may again be performed in regions of the complex plane where the convergence factor is unnecessary.

For $|\eta| \to \infty$ the factors $[1 - \exp(-2\pi|\eta|)]$ in equations (23*a*, *b*) may be replaced by 1. Even for $|\eta| = 1$ the deviation from unity is only 0·25%. We thus obtain

$$f(\eta\to\infty) = \frac{1}{\mathrm{i}k} \lim_{\alpha\to+0} \int_{-\infty}^{\infty} \lambda P^{-}_{\lambda-\frac{1}{2}+\mathrm{i}\epsilon}(\cos\theta) S'_{\lambda-\frac{1}{2}}\,\mathrm{d}\lambda \tag{27}$$

and

$$f(\eta\to-\infty) = \frac{1}{\mathrm{i}k} \lim_{\alpha\to+0} \int_{-\infty}^{\infty} \lambda P^{+}_{\lambda-\frac{1}{2}-\mathrm{i}\epsilon}(\cos\theta) S'_{\lambda-\frac{1}{2}}\,\mathrm{d}\lambda. \tag{28}$$

We should, however, remember that these expressions underestimate the Coulomb amplitude by a factor $2\pi|\eta|$ for $2\pi|\eta| \ll 1$.

In the semiclassical limit equation (18) gives, for λ on or near the real axis,

$$\bar{S}_{\lambda-\frac{1}{2}}(\eta\to\infty) = S_{\lambda-\frac{1}{2}} \tag{29}$$

and

$$\bar{S}_{\lambda-\frac{1}{2}}(\eta\to-\infty) = -\exp(2\pi\mathrm{i}\lambda) S_{\lambda-\frac{1}{2}}. \tag{30}$$

Using equation (19) these immediately give for $\eta > 0$

$$S_{-\lambda-\frac{1}{2}} = \exp(-2\pi i\lambda) S_{\lambda-\frac{1}{2}} \tag{31}$$

and for $\eta < 0$

$$S_{-\lambda-\frac{1}{2}} = \exp(2\pi i\lambda) S_{\lambda-\frac{1}{2}}. \tag{32}$$

Taking the usual relation between the deflection function and the phase of S we find for $\eta > 0$

$$\Theta(-\lambda) = -\Theta(\lambda) + 2\pi \tag{33}$$

and for $\eta < 0$

$$\Theta(-\lambda) = -\Theta(\lambda) - 2\pi. \tag{34}$$

These equations give the well known results $\Theta(0) = \pm\pi$ respectively and also tell us how to interpret the deflection function for negative classical angular momenta in a manner consistent with the analyticity of S.

Equations (27) and (28) are very similar to equations (11a, b) except for those portions of the integrals between $-\infty$ and 0, and as we have already stated the lower limits of equations (11a, b) are usually extended to $-\infty$ anyway. We can now find the significance of these negative λ contributions in terms of the original Poisson formula (6). To do this we again introduce the approximate functions $\tilde{P}^{\pm}_{\lambda-\frac{1}{2}}(\cos\theta)$. (Noting that in equations (27) and (28) we may deform the integration contours away from the origin avoiding the use of these functions for small λ.) Since the functions contain a factor $\lambda^{-1/2}$ the origin is a branch point and we introduce a cut along the negative real axis. It then follows that for real positive λ

$$\tilde{P}^{-}_{-\lambda-\frac{1}{2}+i\epsilon} = \tilde{P}^{+}_{\lambda-\frac{1}{2}} \tag{35}$$

and

$$\tilde{P}^{+}_{-\lambda-\frac{1}{2}-i\epsilon} = \tilde{P}^{-}_{\lambda-\frac{1}{2}}. \tag{36}$$

Equations (27) and (28) may then be written (again dropping the convergence factor)

$$f(\eta > 0) = \frac{1}{ik}\int_0^{\infty} \lambda S_{\lambda-\frac{1}{2}}(\tilde{P}^{-}_{\lambda-\frac{1}{2}} - \exp(-2\pi i\lambda)\tilde{P}^{+}_{\lambda-\frac{1}{2}})\, d\lambda = f_0^{-} - f_{-1}^{+} \tag{37}$$

and

$$f(\eta < 0) = \frac{1}{ik}\int_0^{\infty} \lambda S_{\lambda-\frac{1}{2}}(\tilde{P}^{+}_{\lambda-\frac{1}{2}} - \exp(2\pi i\lambda)\tilde{P}^{-}_{\lambda-\frac{1}{2}})\, d\lambda = f_0^{+} - f_{+1}^{-}, \tag{38}$$

i.e. those parts of the integrals between $-\infty$ and 0 are just other terms (7b) of the original Poisson formula (6) which were neglected because they possessed no stationary points. These terms are only important at backward angles (for $\eta > 0$, $|f_{-1}^{+}(\pi)| = |f_0^{-}(\pi)|$ and for $\eta < 0$, $|f_{+1}^{-}(\pi)| = |f_0^{+}(\pi)|$) and represent flux 'leaking' from the non-classical regions $|\Theta| > \pi$. Note that as $\lambda \to \infty$ the classical deflection function possesses an infinitely wide 'rainbow' at $\Theta = 0$ which prevents the leaking of flux from other non-classical regions. For the same reason the amplitude diverges as $\theta \to 0$ and the forward angle Rutherford cross section is a perfect example of classical rainbow scattering (Berry 1966).

5. Saddle-point evaluation of $f(\theta)$

An approximation often taken for the Coulomb phase in the semiclassical limit is

$$2\mathrm{i}\sigma(\lambda) = 2\mathrm{i}\sigma(0) + (\lambda + \mathrm{i}\eta)\ln(\lambda + \mathrm{i}\eta) - (\lambda - \mathrm{i}\eta)\ln(\lambda - \mathrm{i}\eta) - 2\mathrm{i}\eta \ln \eta, \tag{39}$$

with $\sigma(0) = \eta(\ln \eta - 1)$. This expression may be obtained from the one-turning-point WKB method by application of the usual Langer transformation (e.g. Berry and Mount 1972) or, more simply, by using the asymptotic approximation $\Gamma(z) \sim (2\pi)^{1/2} \mathrm{e}^{-z} z^{z-1/2}(1 + O(z^{-1}))$ (Abramowitz and Stegun 1965) in the exact expression for $S_{\lambda-\frac{1}{2}}$. It can readily be seen that equation (39) leads to equations (31) or (32) depending on whether η is positive or negative. The expression has the disadvantage that we introduce branch points at $\lambda = \pm\mathrm{i}\eta$, which are associated with the classical phenomenon of 'orbiting' when the WKB phase is calculated in the one-turning-point approximation. These singularities will be discussed elsewhere.

In the semiclassical limit the integrals (27) and (28) can be performed by the method of stationary phase or by the saddle-point method (Rowley and Marty 1976). The expansion about the saddle point automatically gives a convergent integral and we may again drop the convergence factor. For $\eta \to \infty$ we obtain the well known result

$$f(\theta) = -\frac{\eta}{2k \sin^2(\frac{1}{2}\theta)} \exp(2\mathrm{i}\sigma(\Lambda) - \mathrm{i}\Lambda\theta + \tfrac{1}{2}\mathrm{i}\pi), \tag{40}$$

where $\Lambda = \eta \cot(\frac{1}{2}\theta)$. Noting that

$$\begin{aligned} &2\sigma(\Lambda) - \Lambda\theta - 2\sigma(0) \\ &\quad = \int_0^{\Lambda} \Theta \,\mathrm{d}\lambda - \int_0^{\Lambda\theta} \mathrm{d}(\Theta\lambda) = -\int_{\pi}^{\theta} \lambda \,\mathrm{d}\Theta = -2\eta \ln \sin(\tfrac{1}{2}\theta), \end{aligned} \tag{41}$$

we find

$$f(\theta) = \frac{-\eta}{2k \sin^2(\frac{1}{2}\theta)} \exp(2\mathrm{i}\sigma(0) - 2\mathrm{i}\eta \ln \sin(\tfrac{1}{2}\theta) + \tfrac{1}{2}\mathrm{i}\pi). \tag{42}$$

Comparing this with the quantal result given by equation (1) we see that the expression gives the exact Coulomb amplitude in the semiclassical limit since

$$\lim_{\eta\to\infty} (2\sigma(0) + \tfrac{1}{2}\pi - 2\sigma_0) = \lim_{\eta\to\infty} (2\sigma(\tfrac{1}{2}) - 2\sigma_0) = 0. \tag{43}$$

In this equation we have used

$$2\sigma(\tfrac{1}{2}) = 2\sigma(0) + \tfrac{1}{2}\Theta(0) + \tfrac{1}{8}\Theta'(0) + \cdots = 2\sigma(0) + \tfrac{1}{2}\pi + O(\eta^{-1}). \tag{44}$$

Note that an error of $\frac{1}{2}\pi$ in the phase of $f(\theta)$ is made if σ_0 is incorrectly associated with $\sigma(0)$. The corresponding results for $\eta < 0$ may be derived similarly.

6. Generalisation

For any S-matrix satisfying $S_{-l-1} = -S_l$ (odd in $(l + \frac{1}{2})$), equations (14), (15) and (17) are valid. However if $S_{-l-1} = S_l$ (even in $(l + \frac{1}{2})$), we can obtain the analogous results

(henceforth any necessary convergence factors are implicit)

$$2f(\theta)=\frac{1}{2\mathrm{i}k}\sum_{l=0}^{\infty}(2l+1)P_l(\cos\theta)S_l-\frac{1}{2\mathrm{i}k}\sum_{l=-\infty}^{-1}(2l+1)P_l(\cos\theta)S_l \tag{45}$$

$$=-\frac{1}{2k}\int_\Gamma \frac{\lambda P_{\lambda-\frac{1}{2}}(\cos(\pi-\theta))}{\cos\pi\lambda}S_{\lambda-\frac{1}{2}}\,\mathrm{d}\lambda \tag{46}$$

$$=\frac{1}{\mathrm{i}k}\sum_{m=-\infty}^{\infty}(-1)^m\int_{-\infty}^{\infty}\lambda P_{\lambda-\frac{1}{2}}(\cos(\pi-\theta))\exp[\mathrm{i}\pi(\lambda-\tfrac{1}{2})]S_{\lambda-\frac{1}{2}}\exp(2\pi m\mathrm{i}\lambda)\,\mathrm{d}\lambda. \tag{47}$$

Since we can write any S_l as a sum of two terms which are odd (S_l^-) and even (S_l^+) in $(l+\frac{1}{2})$ we can represent the scattering amplitude as a sum of equation (15) for S_l^- and equation (46) for S_l^+, or equation (17) for S_l^- and equation (47) for S_l^+. Note that in equations (45), (46) and (47) we may retain the complete $[S_l-1]$ or $[S_{\lambda-\frac{1}{2}}-1]$ from equation (2).

In the semiclassical limit the derivative of the phase of S is a well behaved function of λ (for real λ) and on the real axis the only possible odd terms of S must satisfy

$$S^-_{-\lambda-\frac{1}{2}}=\exp(\mp 2\pi\mathrm{i}\lambda)S^-_{\lambda-\frac{1}{2}}. \tag{48}$$

The only even term satisfies

$$S^+_{-\lambda-\frac{1}{2}}=S^+_{\lambda-\frac{1}{2}}. \tag{49}$$

The above S-matrices correspond to $\Theta(0)=\pi$, $-\pi$ and 0 respectively and we shall label then $S(\pi)$, $S(-\pi)$ and $S(0)$.

The amplitudes from $S(\pm\pi)$ may be written (using equation (17) and making the substitution $\lambda\to-\lambda$ in the $m\lessgtr 0$ terms)

$$f(\theta)=\frac{1}{\mathrm{i}k}\sum_{m=0}^{\infty}(-1)^m\int_{-\infty}^{\infty}\lambda P_{\lambda-\frac{1}{2}}(\cos\theta)S_{\lambda-\frac{1}{2}}(\pm\pi)\exp(\pm 2\pi m\mathrm{i}\lambda)\,\mathrm{d}\lambda. \tag{50}$$

For $S(0)$, equation (47) gives

$$f(\theta)=\frac{1}{\mathrm{i}k}\sum_{m=0}^{\infty}(-1)^m\int_{-\infty}^{\infty}\lambda P_{\lambda-\frac{1}{2}}(\cos(\pi-\theta))\exp[\mathrm{i}\pi(\lambda-\tfrac{1}{2})]S_{\lambda-\frac{1}{2}}(0)\exp(2\pi m\mathrm{i}\lambda)\,\mathrm{d}\lambda. \tag{51}$$

These equations may easily be related to the usual semiclassical expressions (9) by making the substitution $\lambda\to-\lambda$ for those parts of the integrals between $-\infty$ and 0 and by introducing $\tilde{P}^{\pm}_{\lambda-\frac{1}{2}}$. However in the present form the equations permit the use of more powerful techniques for determining the relative importance of the various m values.

Note that in the one-turning-point approximation for scattering at an energy E in a potential $V(r)$ we obtain $\Theta(0)=\pi$ if $V(r)>E$ for any r. If the potential is regular at the origin and $E>V(r)$ for all r then $\Theta(0)=0$. The attractive Coulomb potential, being singular at the origin, is an exception to this result and has $\Theta(0)=-\pi$.

It is interesting to note that for a repulsive potential which dominates the centrifugal potential for small r the *exact* S-matrix satisfies $S_{-\lambda-\frac{1}{2}}=S_{\lambda-\frac{1}{2}}\exp(-2\pi\mathrm{i}\lambda)$ (de Alfaro and Regge 1965) in agreement with our semiclassical result. However, no simple relations similar to equations (48) and (49) can be proved from the Schrödinger equation for an arbitrary potential.

7. Conclusions

By introducing analytic continuations for $\mathrm{Re}\,\lambda < 0$ we have derived some exact integral expressions for the Coulomb amplitude. The semiclassical limit then followed naturally from the symmetry properties of the S-matrix without any of the *ad hoc* assumptions of the usual theory. In particular equations (27) and (28) are independent of any stationary phase arguments. The $m \neq 0$ terms are dealt with exactly and $-\infty$ emerges as the correct lower limit to the integrals.

The results easily generalise to any semiclassical S-matrix and yield integral expressions in which the $m \neq 0$ terms may be properly analysed.

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Appendix

Consider the function $f_\alpha(\theta)$ defined by

$$f_\alpha(\theta) = \sum_{l=0}^{\infty} (2l+1)P_l(\cos\theta)[S_l - 1]\exp[-\alpha(l+\tfrac{1}{2})^2], \qquad \text{(A1)}$$

with $S_l = \Gamma(l+1+\mathrm{i}\eta)/\Gamma(l+1-\mathrm{i}\eta)$ and $\alpha > 0$. The sum is clearly absolutely convergent for all $\alpha > 0$ and we may write (Yennie *et al* 1954)

$$\begin{aligned}(1-\cos\theta)f_\alpha(\theta) &= \sum_{l=0}^{\infty} \{(2l+1)[S_l-1]\exp[-\alpha(l+\tfrac{1}{2})^2] - l[S_{l-1}-1]\exp[-\alpha(l-\tfrac{1}{2})^2] \\ &\quad - (l+1)[S_{l+1}-1]\exp[-\alpha(l+\tfrac{3}{2})^2]\}P_l(\cos\theta),\end{aligned} \qquad \text{(A2)}$$

where we have exploited the recurrence relation

$$(l+1)P_{l+1}(\cos\theta) - (2l+1)\cos\theta P_l(\cos\theta) + lP_{l-1}(\cos\theta) = 0. \qquad \text{(A3)}$$

We thus obtain

$$(1-\cos\theta)\lim_{\alpha\to+0} f_\alpha(\theta) = \sum_{l=0}^{\infty} [(2l+1)S_l - lS_{l-1} - (l+1)S_{l+1}]P_l(\cos\theta), \qquad \text{(A4)}$$

where we have removed the convergence factor from the right-hand side of this equation since it is easy to show that the remaining sum is absolutely convergent even for $\alpha = 0$. Note that the above limit is independent of whether the -1 in the square bracket in equation (A1) is present or not. Inserting the explicit form of S_l into equation (A4) we obtain

$$(1-\cos\theta)\lim_{\alpha\to+0} f_\alpha(\theta) = \sum_{l=0}^{\infty} (2l+1)\left[2\eta^2\frac{\Gamma(l+\mathrm{i}\eta)}{\Gamma(l+2+\mathrm{i}\eta)}\right]P_l(\cos\theta). \qquad \text{(A5)}$$

Consider now the Coulomb amplitude $f(\theta)$ given by

$$2ikf(\theta)=\frac{-i\eta}{\sin^2(\frac{1}{2}\theta)}\exp(2i\sigma_0-2i\eta\ \ln\sin(\tfrac{1}{2}\theta))=-i\eta\frac{\Gamma(1+i\eta)}{\Gamma(1-i\eta)}\left(\frac{2}{1-\cos\theta}\right)^{1+i\eta}. \qquad \text{(A6)}$$

If we attempt to make a Legendre polynomial expansion of this expression we find that the expansion coefficients are not well defined due to the singularity in $f(\theta)$ at $\theta=0$. However, the expansion coefficients $(2l+1)a_l$ of the expression

$$2ik(1-\cos\theta)f(\theta)=-2i\eta\frac{\Gamma(1+i\eta)}{\Gamma(1-i\eta)}\left(\frac{2}{1-\cos\theta}\right)^{i\eta} \qquad \text{(A7)}$$

are well defined despite the remaining singularity in the argument. The quantities a_l are easily shown to be just the $2\eta^2\Gamma(l+i\eta)/\Gamma(l+2+i\eta)$ of equation (A5) and, since the summation in this equation is absolutely convergent, we immediately obtain

$$2ik(1-\cos\theta)f(\theta)=\sum_{l=0}^{\infty}(2l+1)\left[2\eta^2\frac{\Gamma(l+i\eta)}{\Gamma(l+2+i\eta)}\right]P_l(\cos\theta)=(1-\cos\theta)\lim_{\alpha\to+0}f_\alpha(\theta). \qquad \text{(A8)}$$

We may, therefore, drop the -1 from the square bracket of equation (A1) and write the Coulomb amplitude as

$$f(\theta)=\frac{1}{2ik}\lim_{\alpha\to+0}f_\alpha(\theta)=\frac{1}{2ik}\lim_{\alpha\to+0}\sum_{l=0}^{\infty}(2l+1)P_l(\cos\theta)\frac{\Gamma(l+1+i\eta)}{\Gamma(l+1-i\eta)}\exp[-\alpha(l+\tfrac{1}{2})^2] \qquad \text{(A9)}$$

for $\theta\neq 0$. This result is not dependent on the particular convergence factor $\exp[-\alpha(l+\frac{1}{2})^2]$ which has been chosen for convenience in the text.

The above proof depends on the fact that the factor $(1-\cos\theta)$ in equations (A2) and (A7) removes the singularity in $|f(\theta)|$ at $\theta=0$. (Yennie *et al* 1954.) The same technique may also be applied (iteratively if necessary) to obtain more rapid convergence of similar partial wave series (e.g. Alder and Pauli 1969).

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