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A complex angular momentum theory of modified Coulomb scattering

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Abstract. This paper develops an exact complex angular momentum (CAM) theory of elastic scattering for a complex optical potential with a Coulombic tail. The present CAM theory avoids complications due to the long range nature of the Coulombic potential in a straightforward way. This is in contrast to the conventional approach in which the partial wave series is divergent and the scattering amplitude $f(\theta)$ is usually decomposed into a pure Coulomb amplitude and a modifying convergent partial wave series. After considering some general properties of the scattering matrix element $S(\lambda)$, the Sommerfeld-Watson transformation together with a travelling wave (near-side far-side) decomposition, is used to obtain an exact representation for $f(\theta)$ in terms of a background integral $f_{B}(\theta)$ and a series of subamplitudes $f_n^{(\pm)}(\theta)$. New exact representations are derived for $f_B(\theta)$ when $S(\lambda)$ possesses local symmetries of the type $S(-\lambda) = S(\lambda) \exp(\pm 2i\pi\lambda)$ and $S(-\lambda) = S(\lambda)$. The subamplitudes $f_n^{(*)}(\theta)$ are contour integrals and are the exact equivalents of the saddle-point integrals that arise in semiclassical theories. The $f_n^{(\pm)}(\theta)$ can also be evaluated in terms of the Regge pole positions and residues of $S(\lambda)$, which allows a flexible representation for $f(\theta)$ to be derived. The exact results obtained in this paper unify the CAM theory of scattering for Coulombic and short range potentials and are especially suitable for the introduction of semiclassical approximations.

1. Introduction

Non-relativistic scattering for pure and modified Coulomb potentials is an old subject, dating back to the early days of quantum mechanics (e.g. Gordon 1928, Mott 1928). The mathematical complications introduced by the long range character of the Coulomb potential have been considered in several recent publications (Gesztesy and Lang 1981, Garibotti *et al* 1980, Rowley 1978, Taylor 1974, Marquez 1972) and are now fairly well understood.

The partial wave approach is of fundamental importance in low and medium energy ion-ion scattering for atomic, molecular, and nuclear collision systems and can be considered to be a formal solution for modified Coulomb scattering. There are, however, serious practical and conceptual limitations with this approach, which are not necessarily related to the presence of a Coulombic tail in the interaction between the colliding particles. It has been well known since the work of Ford and Wheeler (1959), that a major draw-back with a partial wave approach to heavy-particle scattering is its inability to explain simply the underlying dynamical mechanisms responsible for the rich variety of phenomena observed in the cross sections. Instead, concepts such as (complex, semiclassical) trajectories and surface/Regge waves have proven more useful for explaining the physical significance of the scattering data (for a review see Connor 1980). It is the aim of this paper to show how these different theories and concepts for modified Coulomb scattering can be treated in a unified and rigorous way.

We first briefly summarise the relevant equations of the partial wave analysis in order to make the discussion more specific. We write the radial Schrödinger equation as (e.g. Messiah 1970, ch 11):

$$\frac{d^2\psi_l}{dr^2} + \left(k^2 - \frac{2\eta k}{r} - U(r) - \frac{l(l+1)}{r^2}\right)\psi_l = 0,$$
(1.1)

where the Coulombic and centrifugal parts of the interaction have been made explicit, η is the Sommerfeld parameter, k is the wavenumber and l is the angular momentum quantum number. The (modifying) 'short range' potential U(r) is usually a complex valued function of the real radial variable r and piecewise analytic in some region of the complex r plane containing the non-negative real r axis.

Let $\psi_l(r)$ in (1.1) denote the regular solution having the asymptotic form

$$\psi_l(r) \sim \exp[-i(kr - \eta \ln(2kr) - l\pi/2)] - S_l \exp[i(kr - \eta \ln(2kr) - l\pi/2)], \qquad (1.2)$$

where the exponentials represent the Coulomb distorted 'free' waves and S_l , by definition, is the partial wave scattering matrix element. For pure Coulomb scattering $S_l = S_l^C$ with the Coulomb S matrix given by (e.g. Joachain 1983, ch 6):

$$\mathbf{S}_{l}^{C} \equiv \Gamma(l+1+\mathrm{i}\eta)/\Gamma(l+1-\mathrm{i}\eta).$$
(1.3)

The elastic scattering amplitude $f(\theta)$ is usually obtained from

$$f(\theta) = f_{\rm C}(\theta) + f_{\rm M}(\theta) \tag{1.4}$$

where $f_{\rm C}(\theta)$ is the pure Coulomb contribution, given in closed form by (Joachain 1983, ch 6)

$$f_{\rm C}(\theta) = -\eta \frac{\Gamma(1+i\eta)}{\Gamma(1-i\eta)} \frac{\exp\{-i\eta \ln[\sin^2(\theta/2)]\}}{2k \sin^2(\theta/2)},\tag{1.5}$$

and where the modifying component $f_{M}(\theta)$ is calculated from the partial wave series

$$f_{\mathsf{M}}(\theta) = \frac{\mathrm{i}}{k} \sum_{l=0}^{\infty} (l + \frac{1}{2}) (S_l^{\mathsf{C}} - S_l) P_l(\cos \theta).$$
(1.6)

It is thereby assumed that

$$S_l \underset{l \to \infty}{\sim} S_l^{\mathsf{C}} + \mathrm{o}(l^{-3/2}), \tag{1.7}$$

which is satisfied by a large class of 'short range' potentials. Knowing the scattering amplitude $f(\theta)$, the differential cross section $I(\theta)$ is simply obtained from

$$I(\theta) = |f(\theta)|^2.$$
(1.8)

The decomposition of the scattering amplitude into a Coulomb part and a modifying part in equation (1.4) is due to mathematical rather than physical reasons. The usual partial wave analysis, as it is applicable to non-Coulombic (i.e. $\eta = 0$) potentials, gives the amplitude in the familiar form

$$f(\theta) = \frac{i}{k} \sum_{l=0}^{\infty} (l + \frac{1}{2})(1 - S_l) P_l(\cos \theta).$$
(1.9)

Unfortunately, equation (1.9) is sometimes erroneously claimed to be valid in the usual sense for long range potentials (i.e. $\eta \neq 0$), even if it is straightforward to prove that the sum is divergent (see, e.g., Taylor (1974), and for an excellent historical account see Marquez (1972)). It has recently been shown that equation (1.9) is in fact convergent in a distributional sense (Taylor 1974). More importantly the partial wave series (1.9) exists as an Abel sum (Gesztesy and Lang 1981). The justification of other practical techniques (Mott 1928, Yennie *et al* 1954, Rowley 1978, Garibotti *et al* 1980), to obtain from the divergent series (1.9) a convergent one, is merely a consequence of the Abel summability. Hence, a regularised way of defining the modified Coulomb amplitude is given by

$$f(\theta) = \lim_{\varepsilon \to +0} \frac{\mathrm{i}}{k} \sum_{l=0}^{\infty} (l + \frac{1}{2})(1 - S_l) D_l(\varepsilon) P_l(\cos \theta), \qquad (1.10)$$

where the factor $D_l(\varepsilon)$ acts as a smooth cut-off function for large partial waves. It is essential to have a smooth cut-off (Marquez 1972), but the precise shape is not important (Rowley 1978). For our particular purpose, which is entirely formal, it will be convenient to choose the form (Inopin and Shebeko 1970, Kotlyar and Shebeko 1981)

$$D_l(\varepsilon) = \exp[-\varepsilon(l+1/2)], \qquad \varepsilon > 0. \tag{1.11}$$

A safe way to avoid any problems of convergence (such as the limiting procedure in equation (1.10)) is, of course, to rely on the familiar equations (1.4)-(1.6). The price one has to pay for this (conventional) convergent theory is the introduction of the two unphysical amplitudes $f_{\rm C}(\theta)$ and $f_{\rm M}(\theta)$. We shall see in § 3 that the defects associated with the formulations (1.4) and (1.10) disappear in an exact complex angular momentum (CAM) representation of the amplitude $f(\theta)$. This CAM representation turns out to be formally unaffected by the presence of a Coulombic term in the potential, which means that convergence problems and artificial decompositions do not appear. A similar alternative exact approach for pure Coulomb potentials has been discussed by Rowley (1978) and related approximate theories have been presented by, for example, Knoll and Schaeffer (1976) and Rowley and Marty (1976).

In contrast to many recent theories, particularly in nuclear physics and heavy-ion scattering, where a parametrised S matrix is assumed (Frahn 1980, Frahn and Rehm 1978, Fuller and Moffa 1976, Kauffmann 1977, Shastry and Satpathy 1981), we shall instead adopt the philosophy that a local optical potential is known, so that the properties of the S matrix rigorously follow from that potential through the radial equation (1.1).

Utilising the analytic behaviour of S_l in the CAM plane, we exactly transform $f(\theta)$ into a series of subamplitudes, each carrying the contribution from a specific physical 'mechanism'. By 'mechanism' we mean here the underlying cause of, for example, such well known features as rainbows (of various complexities), orbiting, tunnelling resonances and diffraction (Nörenberg and Weidenmüller 1976, Connor 1980, Child 1984).

Some of the important phenomena just mentioned are closely identified with semiclassical terminology. In the present exact CAM formulation they are represented by contour integrals confined to the half-plane $\operatorname{Re}(l+\frac{1}{2}) \ge 0$. The use of rigorous asymptotic techniques (Gross 1976, Olver 1974) and catastrophe theory (Poston and Stewart 1978) provide a powerful link between, on the one hand, the properties of these contour integrals and, on the other hand, the classification and understanding

of the corresponding mechanism. There are also scattering features of a more wave-like nature, which are conveniently accounted for by the CAM (Regge) poles.

We hope that our contribution to the CAM theory can form a rigorous basis for an improved understanding of the link between structures in cross sections and the topology of the (complex) potential curves, whenever the notion of a local potential is meaningful.

This paper is organised as follows. In § 2 we discuss how the scattering matrix element S_l can be analytically continued into the complex domain $\operatorname{Re}(l+\frac{1}{2}) \ge 0$ and we study its general behaviour. Special attention is paid to 'local' and 'global' symmetries. We also consider the effect of singular potentials of the Lennard-Jones type on the symmetry properties of S_l . With the aid of well known analytic properties of Legendre functions of complex degree, we then exactly transform the partial wave series representation of the scattering amplitude into a series of subamplitudes in § 3, where we also discuss the properties of the transformed amplitude. Our conclusions are given in § 4.

2. Analytic properties of the scattering matrix

2.1. Introduction

A complex angular momentum (CAM) transformation of the scattering amplitude $f(\theta)$ requires the analytic continuation of S_i . The continuation of the Legendre polynomials $P_i(\cos \theta)$ into the CAM plane is standard (e.g. Erdélyi 1953, Robin 1958) and the relations we need will be quoted in § 3 without derivation.

There is a certain arbitrariness, in general, in continuing the discrete set of complex values S_l to form an analytic function $S(\lambda)$ of the complex variable $\lambda \equiv l + \frac{1}{2}$ (de Alfaro and Regge 1965). In the present paper we shall define $S(\lambda)$ by analytic continuation of the corresponding radial Schrödinger equation (1.1) and its regular solution satisfying (1.2), where now l is complex valued.

2.2. Pure Coulomb scattering

For the Coulomb scattering matrix element S_i^C the situation is particularly simple because an analytic closed form solution is available (Joachain 1983, ch 6). Hence, we shall first study the special case $S_l \equiv S_i^C$. From equation (1.3) and elementary properties of Euler's gamma function (Davis 1965) it follows that $S^C(\lambda)$ is free of poles in the half-plane Re $\lambda \ge 0$. Furthermore, from Stirling's formula (Jeffreys and Swirles 1972, p 467, equation (9)):

$$\Gamma(1+z) \sim (2\pi)^{1/2} \exp[(z+\frac{1}{2})\ln(z+\frac{1}{2}) - (z+\frac{1}{2})], \qquad (2.1)$$

it follows that asymptotically

$$S^{C}(\lambda) \sim_{|\lambda| \to \infty} \lambda^{2i\eta}, \qquad \text{Re } \lambda \ge 0,$$
 (2.2)

where η is the Sommerfeld parameter. The modulus of $S^{C}(\lambda)$ is given by

$$|S^{C}(\lambda)| \underset{|\lambda| \to \infty}{\sim} \exp(-2\eta \arg \lambda),$$
 (2.3)

with

$$-\pi/2 \le \arg \lambda \le \pi/2. \tag{2.4}$$

The relations (2.3) and (2.4) imply the following asymptotic behaviour for $|S^{C}(\lambda)|$ along the imaginary λ axis

$$|S^{C}(\lambda)| \underset{|\lambda| \to \infty}{\sim} \begin{cases} \exp(-\pi\eta), & \lambda = \mathbf{i}|\lambda| \\ \exp(\pi\eta), & \lambda = -\mathbf{i}|\lambda|. \end{cases}$$
(2.5)

Recalling that $\eta \equiv Z_1 Z_2 e^2 / \hbar v$, with obvious notation, we conclude that the behaviour along the imaginary λ axis may vary quite strongly from one Coulomb system to another. For example, the heavy-ion nuclear collision ²⁸Si+¹⁶O at ~35 MeV has $\eta \approx 9.5$, whereas for 20 MeV p+p collisions, $\eta \approx 0.025$. The two multiply charged atomic-ion collisions N²⁺ + H⁺ and Ar¹⁸⁺ + H⁻, at 1 eV yield $\eta \approx 300$ and $\eta \approx -2800$, respectively. For the transformations in § 3, however, it will suffice to know that the right-hand side of (2.5) is independent of λ and hence equal to a finite constant.

Before discussing the most general properties of the scattering matrix $S(\lambda)$, it is useful to study in more detail the symmetries of $S^{C}(\lambda)$. By doing so, one can learn much about $S(\lambda)$ itself in those regions of the complex λ plane dominated by the Coulomb potential.

Using the relation (Davis 1965, formula 6.1.17):

$$\Gamma(\frac{1}{2}+z)\Gamma(\frac{1}{2}-z) = \pi/\cos(\pi z),$$
(2.6)

in equation (1.3), gives the global reflection symmetry relation

$$S^{C}(-\lambda) = S^{C}(\lambda) \frac{\exp(i\pi\lambda) \exp(-\pi\eta) + \exp(-i\pi\lambda) \exp(\pi\eta)}{\exp(i\pi\lambda) \exp(\pi\eta) + \exp(-i\pi\lambda) \exp(-\pi\eta)}.$$
 (2.7)

Three limiting cases are apparent

(a) Strong Coulomb repulsion limit

$$S^{C}(-\lambda) = S^{C}(\lambda) \exp(-2i\pi\lambda), \qquad \eta \to +\infty.$$
 (2.8)

(b) Weak Coulomb limit

$$S^{\rm C}(-\lambda) = S^{\rm C}(\lambda), \qquad \eta \to 0.$$
 (2.9)

(c) Strong Coulomb attraction limit

$$S^{C}(-\lambda) = S^{C}(\lambda) \exp(2i\pi\lambda), \qquad \eta \to -\infty.$$
 (2.10)

The usefulness of knowing these three symmetry limits will become evident in § 3 when dealing with the background integral and its physical interpretation. A few remarks should, however, be made at this point. Neither of the symmetries (2.8) and (2.10) is globally valid for a pure Coulomb interaction, but may be approximately satisfied in a large region of the λ plane about the origin $\lambda = 0$. Although the weak Coulomb limit does exist, it is trivial and uninteresting since $S^{C}(\lambda) \equiv 1$ there (cf equation (1.3)). It is not known to the authors what types of potentials (if any) satisfy the symmetries (2.9) and (2.10) exactly. But it is interesting to note that (2.8) is globally valid for $S(\lambda)$ if the potential is singular at the origin r = 0 (see below). This class of potentials is very large (Frank *et al* 1971) and in atomic and molecular scattering includes the familiar Lennard-Jones potentials: $U(r) = gr^{-m} - hr^{-n}$, m > n > 2. Here g and h can be complex coupling constants (except for g = -|g|) without the reflection symmetry (2.8) being broken (Thylwe 1983a).

A straightforward semiclassical analysis of the three symmetries, using the notion of a deflection function $\Theta(\lambda) \equiv (1/2i)(d/d\lambda)[\ln S(\lambda)]$, reveals different behaviour for 'head-on' ($\lambda = 0$) collisions: $\Theta(0) = \pi$, 0 and $-\pi$, corresponding to (2.8), (2.9) and (2.10) respectively (Rowley 1978). The classical conclusion must obviously be that (2.8) holds for potentials with a non-penetrable repulsive core, while (2.9) corresponds to potentials which cannot produce backward reflection at any energy in a head-on collision. The third symmetry (2.10) is unlikely to be valid globally for any realistic class of potentials, because for $\Theta(0) = -\pi$ to hold at all scattering energies, we must have confinement, which is a contradiction.

2.3. Properties of $S(\lambda)$ for a general potential with a Coulombic tail

Next we consider some easily established properties of $S(\lambda)$ for a general potential with a Coulomb tail. As mentioned above, one case where an exact global symmetry relation exists is for a singular potential (de Alfaro and Regge 1965, Frank *et al* 1971). This result is not affected by the presence of a Coulomb component in the potential. We shall not present the proof here, since it is analogous to the derivation given below for other symmetry properties (see also Thylwe 1983a). Thus we merely state the result below.

If $r^2 U(r) \rightarrow \infty$, as $r \rightarrow +0$, and U(r) is not purely attractive at the origin, then

$$S(-\lambda) = S(\lambda) \exp(-2i\pi\lambda)$$
(2.11)

without restriction in the complex λ plane.

Another relation of interest is the so-called extended unitarity symmetry relation. Consider the radial Schrödinger equation (1.1) written in the notation $\lambda \equiv l + \frac{1}{2}$:

$$\frac{d^2\psi_{\lambda}}{dr^2} + \left(k^2 - \frac{2\eta k}{r} - U(r) - \frac{(\lambda^2 - \frac{1}{4})}{r^2}\right)\psi_{\lambda} = 0$$
(2.12)

with the boundary conditions

$$\psi_{\lambda}(0) = 0 \tag{2.13}$$

$$\psi_{\lambda}(r) \sim \exp[-i\kappa(r) + i\lambda\pi/2] - S(\lambda) \exp[i\kappa(r) - i\lambda\pi/2], \qquad (2.14)$$

where we have introduced a symbol $\kappa(r)$ through $\kappa(r) \equiv kr - \eta \ln(2kr) + \pi/4$, for the sake of convenience. Let us also define a particular regular wavefunction $\hat{\psi}_{\lambda}(r)$, which is a solution of the Schrödinger equation with the potential U(r) replaced by its complex conjugate $U^*(r)$, i.e.

$$\frac{d^2\hat{\psi}_{\lambda}}{dr^2} + \left(k^2 - \frac{2\eta k}{r} - U^*(r) - \frac{(\lambda^2 - \frac{1}{4})}{r^2}\right)\hat{\psi}_{\lambda}(r) = 0, \qquad (2.15)$$

with

$$\widehat{\psi}_{\lambda}(0) = 0, \tag{2.16}$$

$$\hat{\psi}_{\lambda}(r) \sim \exp[-i\kappa(r) + i\lambda\pi/2] - \hat{S}(\lambda) \exp[i\kappa(r) - i\lambda\pi/2].$$
(2.17)

 $\hat{S}(\lambda)$ is the scattering matrix element for the potential $2\eta k/r + U^*(r)$. Next we observe

that $\hat{\psi}_{\lambda}^{*}(r)$ and $\psi_{\lambda}(r)$ are both regular solutions satisfying the same differential equation; hence they must be proportional to one another. The proportionality factor is determined by comparison of the asymptotic wavefunctions, with the result that

$$\hat{\psi}_{\lambda^*}^*(r) = -\hat{S}^*(\lambda^*)\psi_{\lambda}(r), \qquad (2.18)$$

and hence

$$\hat{S}^*(\lambda^*)S(\lambda) = 1. \tag{2.19}$$

The extended unitarity symmetry (2.19) for a complex short range potential U(r), in the presence of a Coulomb term, is formally equivalent to the non-Coulombic case (cf equation (3.18) in Thylwe 1983a). Such a symmetry establishes a unique correspondence between the poles and zeros of the scattering matrix when optical potentials are used. Equation (2.19) reduces to the well known result

$$S^*(\lambda^*)S(\lambda) = 1, \qquad U^*(r) \equiv U(r) \tag{2.20}$$

for a real potential.

We now discuss briefly the location of the poles and zeros of $S(\lambda)$ in the half-plane $\text{Re}\lambda \ge 0$. It will turn out that the introduction of a Coulomb tail in the full potential does not alter the fundamental theorems already established for short range interactions (de Alfaro and Regge 1965, Newton 1964, Connor 1975, Thylwe 1983a). It is straightforward to construct from (2.12) and its complex conjugate, the equality

$$\frac{\mathrm{d}}{\mathrm{d}r}\left(\psi_{\lambda}^{*}\psi_{\lambda}^{\prime}-\psi_{\lambda}\psi_{\lambda}^{*\prime}\right)=2\mathrm{i}\,\mathrm{Im}\left(U(r)+\frac{(\lambda^{2}-\frac{1}{4})}{r^{2}}\right)|\psi_{\lambda}|^{2},\tag{2.21}$$

which, with the aid of (2.13) and (2.14), and their complex conjugates, leads to the important relation:

$$|S(\lambda)|^{2} = \exp(-2\pi \operatorname{Im}\lambda) + k^{-1} \exp(-\pi \operatorname{Im}\lambda) \int_{0}^{\infty} [\operatorname{Im} U(r) + 2\operatorname{Re}\lambda \operatorname{Im}\lambda/r^{2}] |\psi_{\lambda}|^{2} dr.$$
(2.22)

From (2.22) we make the following observation: if, for a given λ such that Im $\lambda \leq 0$ (and Re $\lambda > 0$), the potential U(r) in (2.12) satisfies the condition

$$\int_{0}^{\infty} \operatorname{Im} U(r) |\psi_{\lambda}|^{2} \, \mathrm{d}r \leq 0, \qquad (2.23)$$

then we have

$$|S(\lambda)| \le \exp(-\pi \operatorname{Im} \lambda). \tag{2.24}$$

The modulus of $S(\lambda)$ is, consequently, bounded for finite Im λ in the fourth quadrant and has no poles there. The poles (if any) present in the half-plane Re $\lambda > 0$ must therefore lie in the first quadrant. It is not possible, however, to restrict the zeros of $S(\lambda)$ to the fourth quadrant, as would be true for real or emittive (Im U(r) > 0) potentials.

Most of the results discussed above are important for understanding the transformations made in the next section. It is also necessary to make some additional assumptions, which we shall merely suppose to be true and realistic for many situations (de Alfaro and Regge 1965), i.e.

(i) $S(\lambda)$ is meromorphic with simple poles in the half-plane Re $\lambda \ge 0$.

(ii) $|S(\lambda)|$ is bounded from above as $|\lambda| \rightarrow \infty$ in some compact sector $|\arg \lambda| \leq \alpha$ with $0 < \alpha \leq \pi/2$, containing the positive real λ axis.

When $\alpha \neq \pi/2$ in (ii) it is also convenient to make an assumption about the asymptotic behaviour of $S(\lambda)$ along the positive imaginary axis:

(iii) $|S(\lambda)|$ is bounded from above as $|\lambda| \rightarrow \infty$ along the positive imaginary λ axis. For a pure Coulomb potential, relations (2.3)-(2.5) imply we can choose $\alpha = \pi/2$ in (ii) so that the corresponding sector actually coincides with the half-plane Re $\lambda \ge 0$. It is clear that assumption (iii) is superfluous in such a situation. However, if a singular potential is present we expect from non-Coulombic scattering theory that an infinite number of CAM poles and zeros lie along strings extending to infinity in the first and fourth quadrants respectively (e.g. Brander 1966, Frank *et al* 1971, Connor *et al* 1979). In this case α cannot be chosen equal to $\pi/2$ and assumption (iii) provides additional information on the asymptotic behaviour of $S(\lambda)$. It can be checked from relations (2.5) and (2.24) that assumption (iii) is consistent with the known properties of $S(\lambda)$ for pure Coulomb and singular potentials.

3. Transformation of the scattering amplitude

The starting point for our transformation of $f(\theta)$ is equations (1.10) and (1.11). We make this choice because the derivation is then straightforward and concise. For the same reason, we employ the Sommerfeld-Watson transformation (e.g. Newton 1964) rather than the Poisson sum formula (Morse and Feshbach 1953, p 466).

Applying the Sommerfeld-Watson transform to the partial wave series (1.10) and (1.11) results in the contour integral

$$f(\theta) = \lim_{\epsilon \to +0} -\frac{1}{2k} \int_C [S(\lambda) - 1] \frac{\exp(-\epsilon\lambda)}{\cos(\pi\lambda)} P_{\lambda - 1/2}(-\cos\theta)\lambda \, d\lambda, \qquad (3.1)$$

where the contour C encloses the physical angular momentum quantum numbers l=0, 1, ... in the negative (clockwise) sense (see figure 1). In (3.1) we have made use



Figure 1. The complex λ plane and the contour C used in the Sommerfeld-Watson transformation.

of the standard complex continuation of the Legendre polynomials, based on Legendre's differential equation. The resulting Legendre functions of the first kind of complex degree are entire analytic in the half-plane Re $\lambda \ge 0$, with asymptotic behaviour for $|\lambda| \sin \phi \rightarrow +\infty$

$$P_{l}(\cos \phi) \equiv P_{\lambda - 1/2}(\cos \phi) \sim (2\pi\lambda \sin \phi)^{-1/2} \{ \exp[i(\lambda\phi - \pi/4)] + \exp[-i(\lambda\phi - \pi/4)] \}.$$
(3.2)

An inspection of equations (1.11), (2.2) and (3.2), together with the basic assumptions (2.ii) and (2.iii), reveals that the convergence of the integral in (3.1) depends on the fact that the cut-off parameter ε is positive. We therefore cannot interchange the limiting and integration procedures. The situation becomes quite different, as we shall see below when the asymptotic parts of C are deformed away from the real λ axis.

The lower part (Im $\lambda \leq 0$) of the contour C can, with the aid of assumption (2.ii) in § 2, be deformed to approach infinity so that Im $\lambda \rightarrow -\infty$ in the fourth quadrant. A similar shift can be performed in the first quadrant if we ensure that all the poles of $S(\lambda)$ are to the left of the contour. The resulting contour C' is indicated in figure 2. At this point we can take the limit $\varepsilon \rightarrow +0$ since the integral is now convergent.



Figure 2. The contours C', Ω and Γ in the complex λ plane. The crosses and open circles indicate the positions of the poles and zeros of $S(\lambda)$ respectively.

In order to isolate the contribution from the CAM poles, we have to construct a contour by adding and subtracting a contribution along the positive imaginary axis. According to figure 2, we may then split the integral into two parts: one part is defined on a non-closeable path Γ , and the other part is defined on a contour Ω which essentially surrounds the poles in the first quadrant.

Once this decomposition of the scattering amplitude $f(\theta)$ into $\int_{\Gamma} d\lambda + \int_{\Omega} d\lambda$ is completed, the non-dynamical contribution in each integrand can be eliminated. Along Ω , since the integrand has no poles enclosed by the contour we have

$$\frac{1}{2k} \int_{\Omega} P_{\lambda - 1/2}(-\cos \theta) \frac{\lambda}{\cos(\pi \lambda)} \, \mathrm{d}\lambda \equiv 0.$$
(3.3)

From the odd symmetry of the integrand it also follows that

$$\frac{1}{2k} \int_{-i\infty}^{+i\infty} P_{\lambda-1/2}(-\cos\theta) \frac{\lambda}{\cos(\pi\lambda)} d\lambda = -\frac{1}{2k} \int_{\Gamma} P_{\lambda-1/2}(-\cos\theta) \frac{\lambda}{\cos(\pi\lambda)} d\lambda \equiv 0.$$
(3.4)

Hence the scattering amplitude can be written in the form

$$f(\theta) = \frac{1}{2k} \int_{\Gamma} S(\lambda) P_{\lambda-1/2}(-\cos \theta) \frac{\lambda}{\cos(\pi\lambda)} d\lambda - \frac{1}{2k} \int_{\Omega} S(\lambda) P_{\lambda-1/2}(-\cos \theta) \frac{\lambda}{\cos(\pi\lambda)} d\lambda.$$
(3.5)

The evaluation of the second integral in (3.5), using the residue theorem, we uld give us the familiar 'backspace' Regge pole representation (e.g. Newton 1964). However, instead of doing this, it will prove more useful to analyse the terms in (3.5) with semiclassical considerations in mind.

In the following manipulations, we shall make frequent use of the travelling wave decomposition (Nussenzveig 1965, Fuller 1975) of the Legendre functions (Robin 1958), i.e.

$$P_{\lambda-1/2}(\cos\,\theta) \equiv Q_{\lambda-1/2}^{(-)}(\cos\,\theta) + Q_{\lambda-1/2}^{(+)}(\cos\,\theta), \tag{3.6}$$

where, for large $|\lambda \sin \theta|$,

$$Q_{\lambda-1/2}^{(\pm)}(\cos\theta) \sim (2\pi\lambda\,\sin\theta)^{-1/2}\exp[\pm i(\lambda\theta - \pi/4)]. \tag{3.7}$$

In terms of the Legendre function of the second kind $Q_{\lambda-1/2}(\cos \theta)$, these travelling angular waves are defined by

$$Q_{\lambda-1/2}^{(\pm)}(\cos\theta) \equiv \frac{1}{2}(P_{\lambda-1/2}(\cos\theta) \mp (2i/\pi)Q_{\lambda-1/2}(\cos\theta)).$$
(3.8)

The Legendre function $P_{\lambda-1/2}(-\cos\theta)$ can be shown to have the decomposition

$$P_{\lambda-1/2}(-\cos\theta) = iQ_{\lambda-1/2}^{(+)}(\cos\theta) e^{-i\pi\lambda} - iQ_{\lambda-1/2}^{(-)}(\cos\theta) e^{i\pi\lambda}.$$
(3.9)

Note also that $P_{\lambda-1/2}(\cos \theta)$ is singular for $\theta = \pi$, whilst $Q_{\lambda-1/2}^{(+)}(\cos \theta)$ and $Q_{\lambda-1/2}^{(-)}(\cos \theta)$ are both singular for $\theta = 0, \pi$.

Since the background integral in (3.5) requires a different treatment (see below) we shall first apply (3.9) to the second integral in (3.5). Making use of the identity:

$$\left[\cos(\pi\lambda)\right]^{-1} = 2 e^{i\pi\lambda} \sum_{n=0}^{\infty} (-1)^n e^{2in\pi\lambda}, \qquad \text{Im } \lambda > 0.$$
(3.10)

we arrive at the following general result of the CAM theory:

$$f(\theta) = f_{\mathsf{B}}(\theta) + \sum_{n=1}^{\infty} f_n^{(-)}(\theta) + \sum_{n=0}^{\infty} f_n^{(+)}(\theta), \qquad (3.11)$$

with

$$f_n^{(-)}(\theta) \equiv -\frac{\mathrm{i}}{k} (-1)^n \int_{\Omega} S(\lambda) Q_{\lambda-1/2}^{(-)}(\cos \theta) \exp(2\mathrm{i} n\pi\lambda) \lambda \, \mathrm{d}\lambda, \qquad n \ge 1, \qquad (3.12)$$

$$f_n^{(+)}(\theta) \equiv -\frac{\mathrm{i}}{k} (-1)^n \int_{\Omega} S(\lambda) Q_{\lambda-1/2}^{(+)}(\cos \theta) \exp(2\mathrm{i} n\pi\lambda) \lambda \, \mathrm{d}\lambda, \qquad n \ge 0, \qquad (3.13)$$

$$f_{\rm B}(\theta) \equiv \frac{1}{2k} \int_{\Gamma} S(\lambda) P_{\lambda-1/2}(-\cos \theta) \frac{\lambda}{\cos(\pi \lambda)} d\lambda.$$
(3.14)

The subamplitudes $f_n^{(\pm)}(\theta)$ defined in (3.12) and (3.13) are the exact equivalents of the saddle-point integrals that appear in semiclassical theories (Knoll and Schaeffer 1976, Rowley and Marty 1976, Connor 1980). In particular, the $f_n^{(\pm)}(\theta)$ correspond to (complex) trajectories with a negative deflection, whilst the trajectory directly reflected from the core of the potential (if it exists) is hidden in the background amplitude $f_B(\theta)$ —see below. The superscripts (-) and (+) refer to a 'near-side' and 'far-side' decomposition (Fuller 1975, Hussein and McVoy 1984), respectively, and *n* counts the number of revolutions around the scattering centre. We shall return to discuss these subamplitudes later on, in connection with the introduction of Regge pole contributions into $f(\theta)$.

We shall now try to clarify the hidden physics of the 'background integral' $f_B(\theta)$. It is important to emphasise that $f_B(\theta)$ often makes a significant contribution to the total amplitude $f(\theta)$ for medium- and low-energy heavy-particle scattering processes. For example, pure Coulomb scattering is entirely 'background' scattering. In the limit $S(\lambda) \rightarrow S^C(\lambda)$, i.e. $U(r) \equiv 0$, there are no Regge poles in the half-plane Re $\lambda \ge 0$, and all subamplitudes in (3.11), except $f_B(\theta)$, vanish by Cauchy's theorem. Thus we can derive the CAM representation of the Coulomb amplitude,

$$f_{\rm C}(\theta) = \frac{1}{2k} \int_{\Gamma} S^{\rm C}(\lambda) P_{\lambda-1/2}(-\cos \theta) \frac{\lambda}{\cos(\pi\lambda)} d\lambda, \qquad (3.15)$$

which is exact and well defined (convergent). Since $S^{C}(\lambda)$ is bounded in the half-plane Re $\lambda \ge 0$ (recall equations (2.1)-(2.5)), we may also deform Γ to lie along the imaginary λ axis.

We next discuss the general background amplitude $f_B(\theta)$ in the light of its connection with the Coulomb amplitude. From a semiclassical point of view, $f_B(\theta)$ must carry information about the trajectory contribution that is directly reflected (or attracted) by the potential core if such a contribution exists. This fact becomes evident on writing $f_B(\theta)$ in the alternative form,

$$f_{\rm B}(\theta) = -\frac{\mathrm{i}}{k} \int_{\Gamma} S(\lambda) \left(Q_{\lambda-1/2}^{(-)}(\cos \theta) - \frac{1}{2} \frac{\exp(-\mathrm{i}\pi\lambda)}{\cos(\pi\lambda)} P_{\lambda-1/2}(\cos \theta) \right) \lambda \, \mathrm{d}\lambda \tag{3.16}$$

where the identity

$$P_{\lambda-1/2}(-\cos\theta) = -2i\cos(\pi\lambda)Q_{\lambda-1/2}^{(-)}(\cos\theta) + i\exp(-i\pi\lambda)P_{\lambda-1/2}(\cos\theta)$$

has been used. The first term in (3.16) can be recognised as the exact counterpart of the directly reflected semiclassical scattering contribution from the core of a singular (impenetrable) potential (Connor and Mackay 1978)[†]. For a regular potential this term diverges as $\text{Im } \lambda \rightarrow +\infty$. The divergence is, however, exactly cancelled by the second term in (3.16). In fact, whenever a regular potential possesses a physically significant repulsive core, then the role of the second term is essentially only to cancel the divergence of the first term. This is not immediately obvious from (3.16), since the second integrand is certainly not 'small' in the neighbourhood of the real λ axis.

In equation (15) for -i(i/k) read -(i/k).

Instead, the reason is that $S(\lambda)$ for a regular potential with a physically important repulsive core possesses, on a part of the imaginary axis near the origin, the local strong repulsion reflection symmetry $S(-\lambda) = S(\lambda) \exp(-2i\pi\lambda)$ (cf equations (2.8) and (2.11)).

From equation (3.16) and the even character of both $\cos(\pi\lambda)$ and $P_{\lambda-1/2}(\cos\theta)$, the following modified exact expression can be derived:

$$f_{\rm B}(\theta) = -\frac{\mathrm{i}}{k} \int_{\Gamma_{1,\lambda}} S(\lambda) Q_{\lambda-1/2}^{(-)}(\cos\theta) \lambda \, \mathrm{d}\lambda + \frac{\mathrm{i}}{2k} \int_{\Gamma_{1,\lambda}}^{0} [S(\lambda) - S(-\lambda) \exp(2\mathrm{i}\pi\lambda)] \frac{\exp(-\mathrm{i}\pi\lambda)}{\cos(\pi\lambda)} P_{\lambda-1/2}(\cos\theta) \lambda \, \mathrm{d}\lambda + \frac{1}{2k} \int_{\mathrm{i}\infty}^{\mathrm{i}\Lambda} S(\lambda) P_{\lambda-1/2}(-\cos\theta) \frac{\lambda}{\cos(\pi\lambda)} \, \mathrm{d}\lambda + \frac{\mathrm{i}}{2k} \int_{\Gamma_{-1,\lambda}} S(\lambda) P_{\lambda-1/2}(\cos\theta) \frac{\exp(-\mathrm{i}\pi\lambda)}{\cos(\pi\lambda)} \lambda \, \mathrm{d}\lambda,$$
(3.17)

where the truncated contours $\Gamma_{i\Lambda}$ and $\Gamma_{-i\Lambda}$ are defined in figure 3. If the region of local symmetry is large enough, Λ can be chosen so that $i\Lambda$ is sufficiently far away from the saddle points of the first integral. In addition the symmetry-breaking contribution in the second integral, as well as the tail contribution in the last two integrals, will become insignificant in this situation.

When U(r) contains a singular potential core, no matter how small, the expression (3.17) reduces to the corresponding non-Coulombic result (Connor and Mackay 1978) on letting $\Lambda \rightarrow +\infty$, i.e.



Figure 3. The contours $\Gamma_{i\lambda}$ and $\Gamma_{-i\lambda}$ in the complex λ plane. The crosses and open circles indicate the positions of the poles and zeros of $S(\lambda)$ respectively.

Similarly, one can use the fact that the S matrix may also locally satisfy the reflection symmetries $S(-\lambda) = S(\lambda)$ and $S(-\lambda) = S(\lambda) \exp(2i\pi\lambda)$, in the important region near the origin. Again, the analogy with the pure Coulomb cases in (2.9) and (2.10) means we can derive two alternative exact representations for the background amplitude:

$$f_{\rm B}(\theta) = \frac{1}{2k} \int_{i\Lambda}^{0} [S(\lambda) - S(-\lambda)] P_{\lambda-1/2}(-\cos\theta) \frac{\lambda}{\cos(\pi\lambda)} d\lambda$$
$$+ \frac{1}{2k} \int_{i\infty}^{i\Lambda} S(\lambda) P_{\lambda-1/2}(-\cos\theta) \frac{\lambda}{\cos(\pi\lambda)} d\lambda$$
$$+ \frac{1}{2k} \int_{\Gamma_{-1}}^{\dots} S(\lambda) P_{\lambda-1/2}(-\cos\theta) \frac{\lambda}{\cos(\pi\lambda)} d\lambda, \qquad (3.18)$$

and

$$f_{\rm B}(\theta) = \frac{\mathrm{i}}{k} \int_{\mathrm{i}\infty}^{-\mathrm{i}\Lambda} S(\lambda) Q_{\lambda-1/2}^{(+)}(\cos\theta) \lambda \, \mathrm{d}\lambda$$
$$-\frac{\mathrm{i}}{2k} \int_{0}^{-\mathrm{i}\Lambda} [S(\lambda) - S(-\lambda) \exp(-2\mathrm{i}\pi\lambda)] P_{\lambda-1/2}(\cos\theta) \frac{\exp(\mathrm{i}\pi\lambda)}{\cos(\pi\lambda)} \lambda \, \mathrm{d}\lambda$$
$$+\frac{1}{2k} \int_{\Gamma_{-\mathrm{i}\Lambda}} S(\lambda) P_{\lambda-1/2}(-\cos\theta) \frac{\lambda}{\cos(\pi\lambda)} \, \mathrm{d}\lambda$$
$$-\frac{\mathrm{i}}{2k} \int_{\mathrm{i}\infty}^{\mathrm{i}\Lambda} S(\lambda) P_{\lambda-1/2}(\cos\theta) \frac{\exp(\mathrm{i}\pi\lambda)}{\cos(\pi\lambda)} \lambda \, \mathrm{d}\lambda. \tag{3.19}$$

In the derivation of (3.19) we have made use of the identity

$$Q_{\lambda-1/2}^{(-)}(\cos\theta) = 2\mathrm{i}\cos(\pi\lambda) Q_{\lambda-1/2}^{(+)}(\cos\theta) - \mathrm{i}\exp(\mathrm{i}\pi\lambda) P_{\lambda-1/2}(\cos\theta).$$

The representation (3.18) suggests that $f_B(\theta)$ will be physically insignificant when the local symmetry $S(-\lambda) = S(\lambda)$ holds near the origin. All the important physical effects are then contained in the remaining subamplitudes (3.12) and (3.13). As pointed out in § 2, we cannot give an example of a non-vanishing potential for which this symmetry is satisfied globally. On the other hand, it is trivial to construct a parametrised S matrix with this property (Remler 1971).

When the third kind of local symmetry is present, as for a strong Coulomb attraction (cf equation (2.10)), the representation (3.19) is the relevant one. In this case $f_{\rm B}(\theta)$ corresponds physically to 'attractive' trajectories with winding number n = 0. At first sight it appears that these trajectories are also accounted for by the amplitude $f_0^{(+)}(\theta)$ in (3.11). This apparent double counting of trajectories will now be explained.

Consider as a simple example the pure attractive Coulomb potential. All trajectories are attracted to the scattering centre for such a potential. The classical deflection function increases monotonically from $-\pi$ to 0, as λ moves along the real positive axis. There is no orbiting phenomenon, since no centrifugal barrier exists. Consequently, the only relevant terms in (3.11) are $f_{\rm B}(\theta)$ and $f_{0}^{(+)}(\theta)$. Equations (3.13) and (3.19) show that the integrands for $f_{\rm B}(\theta)$ and $f_{0}^{(+)}(\theta)$ are essentially the same, but the contours of integration are quite different. The behaviour of the deflection function implies there is only one saddle point. This saddle point is passed through twice when evaluating $f_{0}^{(+)}(\theta)$ along the (deformed) contour Ω . Hence $f_{0}^{(+)}(\theta)$ vanishes while $f_{\rm B}(\theta)$ remains. Another way of deciding whether the subamplitudes defined on Ω (i.e. all but $f_B(\theta)$ vanish or not, is to examine the S matrix poles in the CAM plane. If no poles are present in the first quadrant, as is the case for a pure Coulomb potential, then only $f_B(\theta)$ is left.

We shall not attempt to exhaust all conceivable situations where $f_{\rm B}(\theta)$ corresponds to attractive trajectories. The background amplitude $f_{\rm B}(\theta)$ obviously has many hidden, yet physically important properties. A key role for understanding $f_{\rm B}(\theta)$ is the local symmetry of the S matrix, which reflects the classical nature of the potential core (if not too complex), e.g. the behaviour of the deflection function near $\lambda = 0$.

To conclude this section we shall show how the CAM poles can be used to provide an alternative exact description of the subamplitudes $f_n^{(\pm)}(\theta)$. In fact, the integration contour Ω has been constructed so that it can be closed around the S matrix poles making possible an evaluation by residues. It is obvious that this same set of poles can also be used to characterise all of the subamplitudes $f_n^{(\pm)}(\theta)$. Thus if λ_m , $m = 0, 1 \dots$ are the positions in the first quadrant of the poles of the S matrix (finite or infinite in number) and r_m are the corresponding residues, then application of the residue theorem converts (3.12) and (3.13) into

$$f_n^{(\pm)}(\theta) = \frac{2\pi}{k} (-1)^n \sum_{m=0} \lambda_m r_m \exp(2in\pi\lambda_m) Q_{\lambda_m-1/2}^{(\pm)}(\cos\theta).$$
(3.20)

The simple way in which the winding number n enters into equation (3.20) lets us analytically sum as a geometric series (since Im $\lambda_m > 0$) an infinite number of consecutive subamplitudes. Thus

$$f_{P,N_{\pm}}^{(\pm)}(\theta) = \sum_{n=N_{\pm}}^{\infty} f_{n}^{(\pm)}(\theta)$$

= $(-1)^{N_{\pm}} \frac{\pi}{k} \sum_{m=0} \lambda_{m} r_{m} \frac{\exp[i(2N_{\pm}-1)\pi\lambda_{m}]}{\cos(\pi\lambda_{m})} Q_{\lambda_{m}-1/2}^{(\pm)}(\cos\theta)$
 $N_{\pm} \ge 0, N_{\pm} \ge 1.$ (3.21)

The subscript P in (3.21) indicates a pole representation and N_{\pm} is the minimum winding number of the far-side (+) or near-side (-) waves (or trajectories). Because of the factor $\exp[i(2N_{\pm}-1)\pi\lambda_m]$ in the residue series (3.21), it is evidently more difficult to describe phenomena with a small winding number n than those with a large n. Furthermore, for n (or N_{\pm}) fixed, $f_n^{(-)}(\theta)$ and $f_n^{(+)}(\theta)$ converge more rapidly in the forward and backward directions respectively, provided θ is not too close to 0 or π where the $Q_{\lambda m^{-1/2}}^{(\pm)}(\cos \theta)$ are singular. An illustrative example of the convergence properties of $f_0^{(\pm)}(\theta)$ is found in rainbow scattering for non-Coulombic systems (Connor and Jakubetz 1978, Connor et al 1981). Here, only $f_{\rm B}(\theta)$ and $f_0^{(+)}(\theta)$ give a significant contribution in (3.11). The background integral $f_{\rm B}(\theta)$ represents the directly reflected trajectory from the core of the potential and $f_0^{(+)}(\theta)$ can be represented either by a uniform Airy amplitude or a residue sum of the form (3.20). When the scattering possesses a pronounced primary rainbow, the residue series is slowly convergent in the classically allowed range of angles. In contrast to this, CAM pole descriptions have proved to be a particularly elegant and accurate method for describing classically 'forbidden' events involving complex valued classical trajectories (Connor et al 1981), where the Regge poles correspond physically to surface or creeping waves. The CAM theory is also useful for describing scattering when there are a large number of orbiting

trajectories (Korsch and Thylwe 1983, Thylwe 1983b) and for the analysis of tunnelling (shape) resonances (Connor 1972, Connor and Smith 1983).

On combining equations (3.20) and (3.21), the scattering amplitude $f(\theta)$ can be written in the form

$$f(\theta) = f_{\rm B}(\theta) + \sum_{n=1}^{N_{-}-1} f_n^{(-)}(\theta) + \sum_{n=0}^{N_{+}-1} f_n^{(+)}(\theta) + f_{P,N_{-}}^{(-)}(\theta) + f_{P,N_{+}}^{(+)}(\theta).$$
(3.22)

The presence of the integers N_+ and N_- makes this representation particularly flexible. This is a desirable feature in inversion theories for example, where one wants to minimise the total number of significant terms in (3.22). However, it is necessary to remember that each subamplitude, $f_n^{(\pm)}(\theta)$ and/or $f_{P,N_{\pm}}^{(\pm)}(\theta)$, may have several components if there are multiple saddle-points or several contributing pole terms.

4. Concluding remarks

An exact and flexible representation of the scattering amplitude $f(\theta)$ has been derived, which provides a suitable starting point for rigorous and systematic approximation schemes. The present derivation is simpler than that given earlier (Thylwe 1983a), which was restricted to short range potentials. We have shown that the presence of a long range Coulomb tail can be incorporated into the theory and that it does not introduce any essential difficulties.

The CAM formulation removes insignificant contributions from the real l axis. Put in other words, small quantum effects are transferred to the 'tails' of the contour integrals or, if present in the half-plane $\operatorname{Re}(l+1/2) \ge 0$, to the remote CAM poles of the S matrix.

We have discussed the semiclassical aspects of the background amplitude $f_{\rm B}(\theta)$ in the light of local symmetries of the S matrix. One of the reflection symmetries considered is globally valid if the potential contains a singular core.

It is important to realise that our CAM formulation is valid for arbitrarily strong absorption in the optical potential, which is of particular interest for certain heavy ion scattering processes. There is no reason to suppose that the saddle-point integrals arising from the subamplitudes lose their meaning in the presence of strong absorption. On the contrary the CAM theory is likely to be particularly useful in such situations. The l window formalism (Rowley 1980) and other sharp-cut-off theories (see, e.g., Inopin and Shebeko 1970) designed for this type of problem, differ from the CAM approach in one fundamental respect: they explore the S matrix on the real l axis, parametrising its behaviour there with basically real shape parameters. The problem of the divergence of the partial wave series then arises, so that either S_i is split into a pure Coulomb part and a modifying part (Rowley 1980), or else a convergence factor as in equation (1.10) has to be introduced (Inopin and Shebeko 1970, Kotlyar and Shebeko 1981). A noticeable feature of these essentially real angular momentum theories is that it makes sense to rearrange the partial wave sum, or the corresponding Poisson integrals, into a form in which there appears the difference $Z_i \equiv S_i - S_{i-1}$ or the derivative dS/dl, respectively. A similar approach in the CAM formulation would destroy the simplicity of the contour integrals (the corresponding residue series are unaffected) without bringing further insight into the strong absorbtion mechanism. Systematic comparisons of the strengths and weaknesses of these differing theories are, however, lacking at present and a complete discussion of scattering for strong absorption goes beyond the scope of this paper.

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