# Complex-Angular-Momentum Analysis of Atom-Atom Scattering Experiments

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$S$-matrix elements typically encountered in atom-atom scattering may be phenomenologically parametrized using meromorphic functions of complex angular momenta. The contribution to the scattering amplitude of each pole of the $S$ matrix is of such a simple nature (effectively, decaying oscillations for parameters encountered in practice) as to greatly facilitate the deduction of the phase shifts from scattering data. Some of these poles should be close to the true (Regge) poles of the exact $S$ matrix about which much theoretical information is available. There is some discussion outlining how many diverse phenomena such as rainbows, orbiting, and curve crossing can all be parametrized under the same scheme, thus leading to their unified treatment.

## I. INTRODUCTION

Atom-atom scattering at low energies typically involves many hundreds of partial waves. The theoretical analysis of such problems has been dominated by semiclassical considerations. Thus for example, the phase shifts are deduced from potentials via the WKB approximation. Similarly, sums over partial waves are first converted to integrals and then approximated by stationary phase methods.

In a particularly well-known paper[1] written in 1959, Ford and Wheeler discussed in some detail a whole range of semiclassical scattering phenomena. Since that paper there have been many applications, refinements, and extensions of their approach.[2] Just at the time that Ford and Wheeler's paper was being published, the field of high-energy physics was beginning to turn its attention to what has become known as Regge poles. In fact, also in 1959, Regge was motivated to study the general properties of nonrelativistic potential scattering $S$ matrices considered as analytic functions of the angular-momentum variable.[3,4] Although these investigations were not motivated either by semiclassical problems or by problems associated with the handling of many partial waves, they are in fact related by a long and historic line to investigations which were just so motivated. For example, in Sommerfeld's book[5] on partial differential equations, he discusses the Green's function describing radio propagation near the surface of the Earth. He notes that the contribution to this Green's function from about 1000 partial waves is contained in what has come to be known as one Regge-pole contribution. Obviously any mode of analysis which condenses the effect of so many terms into what is in fact a single relatively simple analytic expression may be of great use.

It is the purpose of this paper to indicate how some of the many varied and interesting effects seen in atom-atom scattering experiments may be analyzed using $S$ matrices which are simple analytic functions of complex angular momenta and which involve only a few parameters particular to the system being studied. Further, it will be seen that these parameters can be simply and directly related to the experimental data so that this mode of analysis becomes a useful tool in the attempt to deduce the phase shifts or, equivalently, the potential.

In Sec. II the basic results are derived. In Sec. III a numerical example typical of a system with large slowly varying phase shifts is given and how a more detailed analysis may be performed is discussed. Rapidly changing phases typical of orbiting and level-crossing situations are discussed in Sec. IV. The problem of total-cross-section measurements is touched upon in Sec. V. The particulars of any one type of system have not been investigated in great detail but rather we have attempted to show the great intrinsic range and power of the method.

## II. BASIC RESULTS FOR DIFFERENTIAL CROSS SECTION

We are concerned here with the elastic interaction between two atomic systems at least one of which is uncharged, so that there is a long-range attractive tail and a short-range relatively sharply cutoff repulsive core. It is convenient to treat these two parts in rather different ways and, reflecting this, the phase shift $\eta$ is considered as the sum of two parts

$$\eta = \eta_C + \eta_T , \tag{1}$$

where the subscripts $C$ and $T$ stand for "core" and "tail," respectively.

The (diagonal) $S$-matrix elements in the angular-momentum representation are similarly written as

$$S(\lambda) = e^{2i\eta} = S_C(\lambda)\, S_T(\lambda) = e^{2i\eta_C}\, e^{2i\eta_T} , \tag{2}$$

where we will often use the variable

$$\lambda = l + \tfrac{1}{2}, \quad l = 0, 1, 2, \cdots . \tag{3}$$

Much of the problem with which we are concerned amounts to summing, in an interesting manner, the partial-wave series

$$ikf(\theta) = \sum_\lambda \lambda P_{\lambda-1/2}(x)\,[S(\lambda)-1], \quad x=\cos\theta\ . \tag{4}$$

To do this we decompose the sum into a core and tail part

$$ikf = \sum_\lambda \lambda P_{\lambda-1/2}(x)\,[S_T(S_C-1)+(S_T-1)]$$
$$= ikf_C + ikf_T\ . \tag{5}$$

After these preliminaries, the basic approach of this paper may be discussed. The core phases vanish rapidly beyond some angular momentum called $l_C$. For $l < l_C$, they decreased to large negative values rapidly and monotonically. In this region it will also be seen that the tail phases needed in physically interesting cases vary much more slowly than the core phases so that, qualitatively, $f_C$ is similar to the hard-sphere scattering amplitude. Since the structure of this amplitude is well known[6] and since the number of partial waves needed for its accurate computation is relatively small (compared to that needed to compute $f_T$), it may well turn out to be quite reasonable, in practical cases, to simply compute the sum for $f_C$ by machine. Alternatively, however, we shall discuss simple and standard analytic approximations to this sum.

The case of the tail contribution is quite different. It is impractical and unedifying to sum the large number of partial waves needed to accurately compute $f_T$. Analytic approximations based on the stationary phase approximation have been given.[1,2] In this paper, we indicate another type of analytic approximation which is more general in scope, more accurate in principle, more interesting in theoretical connotations, and possibly somewhat simpler in form.

$S_T$ will be represented by the simplest type of meromorphic function in complex $\lambda$ which is at the same time unitary and symmetric. One writes

$$S_T = \sum_{P=1}^{N} S_P\ , \tag{6}$$

$$S_P = (\lambda^2 - \lambda_P^{*2})/(\lambda^2 - \lambda_P^2)\ . \tag{7}$$

Thus $S_P(\lambda) = S_P(-\lambda)$ for any $\lambda$ and $S_P(\lambda) = [S_P^*(\lambda)]^{-1}$ for real $\lambda$.

The general properties of an $S$ matrix parametrized in this fashion can easily be derived. In particular, one has that the tail phase $\eta_T$ is the sum of contributions, one from each pole with

$$\eta_T = \sum_P \eta_P\ , \tag{8}$$

$$\eta_P = -\arg(\lambda-\lambda_P) - \arg(\lambda+\lambda_P)\ . \tag{9}$$

Similarly, one has for the deflection functions

$$\Theta_T = \sum_P \Theta_P\ , \tag{10}$$

$$\Theta_P = -4\lambda(\mathrm{Im}\lambda_P^2)\,|\lambda^2-\lambda_P^2|^{-2}\ . \tag{11}$$

A pole in the I (and III) quadrant corresponds to attraction and provides a positive monotonically decreasing function of increasing $\lambda$ as its contribution to $\eta$ and vice versa for a repulsive pole. Figure 1 illustrates this and other basic properties of $\theta_P$ and $\eta_P$.

Note in particular the restrictions

$$|\eta_P(0) - \eta_P(\infty)| < \pi\ , \tag{12}$$

$$\Theta_P(0) = 0. \tag{13}$$

Since typically in such systems some tens-of-radians worth of attractive phase shifts are experienced in the tail region, Eq. (12) implies that a few attractive poles will be needed in general. Similarly, repulsive cores force the phase shift to large negative values as $\lambda \to 0$ [$\Theta(0) \cong \pi$] and Eqs. (12) and (13) imply that such being the case, parametrization of these phases would require cumbersomely large numbers of repulsive poles. This is the basic reason the core region is treated by another method in this paper.

It is interesting and appropriate at this point to note that Regge's investigations[3,4,7] give us insight as to why attractive poles are more useful than repulsive poles. He has shown that for Re$\lambda > 0$ the *only* singularities $S(\lambda)$ may have are simple attractive poles. Repulsive poles as defined here do not in fact exist in the exact $S$ matrix; repulsion is due to other singularities in the half-plane Re$\lambda < 0$. However, it still may be useful to phenomenologically simulate at least part of the repulsion with poles.

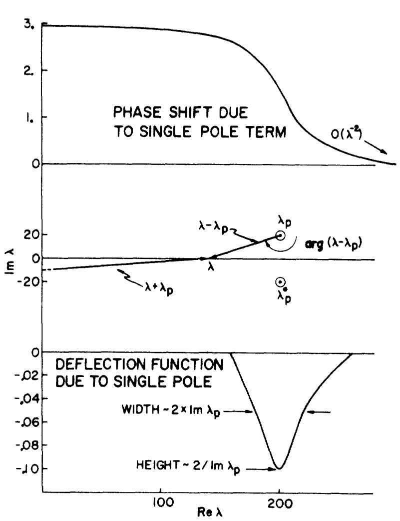


FIG. 1. The effect of a single pole at $\lambda_p = 200 + 20i$. Graphs of $\eta_p$, $\theta_p$, and the complex $\lambda$ plane are stacked on top of one another. Angles are in radians.

The tail amplitude can now be computed *exactly* using the Watson-Sommerfeld transformation

$$ikf_T = \sum_\lambda \lambda P_{\lambda-1/2}(x)(S_T - 1)$$
$$= (2\pi i)^{-1} \oint (\pi/\cos\pi\lambda)\lambda P_{\lambda-1/2}(-x)(S_T-1)d\lambda \ . \tag{14}$$

The contour in complex $\lambda$ encloses clockwise the poles due to $\cos\pi\lambda$. This contour may now be opened up until it stretches along the imaginary axis leaving in the process the contributions due to the poles of $S_T$. The imaginary axis ("background") integral vanishes due to the antisymmetry of the integral—this is the reason for insisting $S_T$ be symmetric in $\lambda$. Thus we have

$$ikf_T = (2\pi i)^{-1} \tfrac{1}{2}\pi \oint d\lambda^2 [P_{\lambda-1/2}(-x)/\cos\pi\lambda]\, S_T$$
$$= \sum_P \tfrac{1}{2}\pi [P_{\lambda P-1/2}(-x)/\cos\pi\lambda_P]\, C_P(\lambda_P^2 - \lambda_P^{*2}) \ , \tag{15}$$

where the integral has now been rewritten as a clockwise circuit about the poles of $S_T$ in the $\lambda^2$ plane. $C_P(\lambda_P^2 - \lambda_P^{*2})$ is the residue of $S_T$ at the $P$th pole using the notation

$$S_T = C_P(\lambda^2) S_P, \quad C_P(\lambda_P^2) = C_P \ , \tag{16}$$

so that the function $C_P(\lambda^2)$ is the cofactor of $S_P$ in $S_T$.

The formula may be clarified by noting a relation between various Legendre functions on the cut,[8,9]

$$\frac{\pi}{2}\frac{P_{\lambda-1/2}(-x)}{\cos\pi\lambda} = Q_{\lambda-1/2}(x+i0)(1+e^{-2\pi i\lambda})^{-1}$$
$$+ Q_{\lambda-1/2}(x-i0)(1+e^{+2\pi i\lambda})^{-1} \ . \tag{17}$$

As long as $|\mathrm{Im}\lambda| \gtrsim 2$, one or the other of these terms will be strongly damped for all $\theta$. The case $|\mathrm{Im}\lambda| \lesssim 2$ corresponds to, in the context of atom-atom scattering, orbiting and will be discussed separately. Thus, except when poles lie exceptionally close to the real axis, one has, to excellent approximation,

$$ikf_T \cong \sum_P C_P(\lambda_P^2 - \lambda_P^{*2}) Q_{\lambda_{P-1/2}}(x - i0_P), \tag{18}$$

$$0_P = 0 \,\mathrm{sgn}(\mathrm{Im}\lambda_P). \tag{19}$$

The great power and simplicity of this formula is further revealed upon noting that for large $\lambda_P$ one has the following rapidly convergent expression[10]:

$$Q_{\lambda-1/2}(\cos\theta \mp i0) = \left(\frac{\pi}{2\sin\theta}\right)^{1/2} \frac{\Gamma(\lambda+\frac{1}{2})}{\Gamma(\lambda+1)} e^{\pm i(\pi/4+\lambda\theta)}$$
$$\times F(\tfrac{1}{2}, \tfrac{1}{2}, 1+\lambda; \zeta_\mp), \quad \zeta_\mp = \mp i e^{\pm i\theta}/2\sin\theta \tag{20}$$

$F$ denoting the hypergeometric function. For $\theta > 30°$, the series converges, while for $\theta \lesssim 30°$ it diverges, but for large $\lambda$ it is an initially rapidly convergent asymptotic series.[11] By inserting an accurate approximation for the $\Gamma$ functions[12] we obtain the final form useful for computation:

$$Q_{\lambda-1/2}(\cos\theta \mp i0) \cong \left(\frac{\pi}{2(\lambda+\frac{1}{4})\sin\theta}\right)^{1/2} \left(1 - \frac{1}{64(\lambda+\frac{1}{4})^2}\right)$$
$$\times e^{\pm i(\pi/4+\lambda\theta)} F_\mp \ , \tag{21}$$

$$F_\mp = \sum_{n=0} f_n \zeta_\mp^n, \quad f_0 = 1, \quad f_n = \frac{(n-\frac{1}{2})^2}{n(n+\lambda)} f_{n-1} \ .$$

Thus, the contribution of a pole is given by, up to a slowly varying factor, the form $\exp(\pm i\,\mathrm{Re}\lambda_P\theta - |\mathrm{Im}\lambda_P|\theta)$—a decaying oscillation in angle, the frequency and decay rate of which are simply related to pole position. The simplicity of this result should make it possible to roughly guess at the pole positions from direct examination of experimental differential-cross-section data. This would be a necessary initial step in a least-squares fit to experiment in an attempt to deduce the $S$ matrix from the cross section.

Another example of this simple correspondence can be seen in the numerical example of Sec. III in which the peak in the deflection function is caused by a group of $N = 10$ poles clustered about $200 + 20i \cong \lambda_P$ (for every $P$). Thus the value of $\theta_T \cong N\theta_P$, at its maximum, when $\lambda^2 \cong \mathrm{Re}\lambda_P^2$, is simply obtained from Eq. (11) to be $2N[(\mathrm{Re}\lambda_P)^2 - (\mathrm{Im}\lambda_P)^2]^{1/2}/(\mathrm{Re}\lambda_P\,\mathrm{Im}\lambda_P)$, which is the classical rainbow angle (in the example this turns out to be close to 1 rad).

An analytic approximation to the core amplitude may be obtained via the saddle-point method. It should be emphasized that it is possible and probably worthwhile in practice to simply sum this series. However, it is useful in any case to see what the general properties of such a sum are from an analytic expression. One writes

$$ikf_C \cong \int_0^{\lambda_C} d\lambda\, \lambda P_{\lambda-1/2}(S_C - 1) \ , \tag{22}$$

$$P_{\lambda-1/2} = (i/\pi)[Q_{\lambda-1/2}(x+i0) - Q_{\lambda-1/2}(x+i0)] \tag{23}$$

$$= q_\lambda^{(-)} e^{-i\lambda\theta} - q_\lambda^{(+)} e^{+i\lambda\theta} \ , \tag{24}$$

where $q_\lambda^{(\pm)}$ are slowly varying in comparison to other factors. This integral has no end-point contribution to first order because $S_c(\lambda_c) = 1$. Thus the main contribution is, as usual,[2] from the stationary phase of

$$\int d\lambda\, \lambda\, q_\lambda^{(-)} e^{-i\lambda\theta} e^{2i\eta}$$
$$\cong \lambda_S q_{\lambda_S}^{(-)} e^{-i\lambda_S\theta} S(\lambda_S) \int d\lambda\, e^{i(1/2)\Theta_S'(\lambda-\lambda_S)^2}$$
$$\cong (i/\pi)\, Q_{\lambda_{S-1/2}}(x+i0)\, \lambda_S S(\lambda_S) e^{-i\pi/4}(2\pi/-\Theta_S')^{1/2} \ , \tag{25}$$

$$2\left.\frac{d\eta}{d\lambda}\right|_{\lambda_S(\theta)} = \theta \ , \tag{26}$$

$$\Theta_S' = 2\left.\frac{d^2\eta}{d\lambda^2}\right|_{\lambda_S} < 0 \ . \tag{27}$$

This must be added to $ikf_T$ to obtain $ikf$ and provides in practice a practically flat hard-core reflection-type amplitude. A numerical example illustrating the use of these results is given in the Sec. III.

## III. NUMERICAL EXAMPLE

As a typical example of the data to which methods may be applied we have taken the results of Champion *et al.*[13] on 6-eV elastic $p+\mathrm{Ar}$ scattering. They find a phase shift which reaches a maximum of about 30 rad at $\lambda \approx 150$ and then decreases monotonically to about $-100$ rad at $\lambda = 0$. The width of the attractive region is about 100 units of angular momentum and the deflection function has a minimum at about $\lambda = 200$. As a rough simulation of this we placed 10 poles close to the point $200+20i$ in the complex $\lambda$ plane (10 poles $\times \sim 3$ rad/pole $\cong 30$ rad). For the hard-core phase shift $\eta_C$ it proved convenient to use the expression

$$\eta_C = \lambda_C \left\{ \frac{\lambda}{\lambda_C} \cos^{-1}\left(\frac{\lambda}{\lambda_C}\right) - \left[1 - \left(\frac{\lambda}{\lambda_C}\right)^2\right]^{1/2} \right\}, \tag{28}$$

which can be obtained by taking the $S$ matrix for hard-sphere scattering ($\lambda_C = k \times$ radius of sphere)

$$S(k, \lambda) = -H_\lambda^{(2)}(\lambda_C)/H_\lambda^{(1)}(\lambda_C) \tag{29}$$

and applying the Debye approximation to the Hankel functions.[6] This approximation is valid except near the edge of the sphere and has the virtue of being simple and accurately simulating small $\lambda$ behavior of $\eta_C$. In the present example we have taken $\lambda_C = 150$. Finally, a single repulsive pole was placed at $\lambda = 200 - 200i$ which had the effect of canceling the asymptotic behavior of the attractive poles causing the phase shift to go as $\lambda^{-4}$ as $\lambda \to \infty$. Because of the large imaginary value of this pole's position it can have essentially no effect on the differential cross section for angles $\theta \gtrsim \frac{1}{200}$ rad.[14]

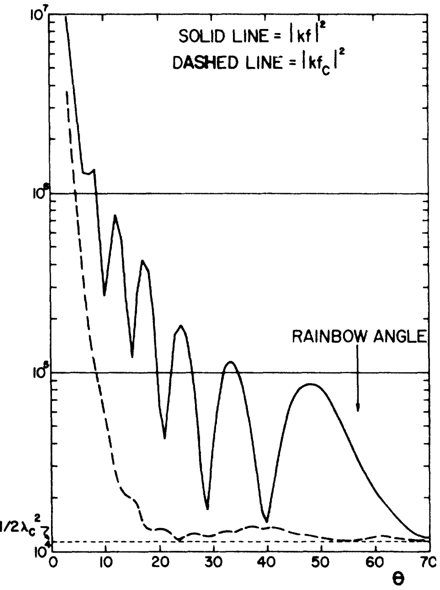


FIG. 3. Smoothed differential cross section due to 10 poles at $\lambda_p = 200 + 20i + \exp[(P/10)2\pi i]$ $P = 1, \ldots 10$ and one at $\lambda_{11} = 200 - 200i$ plus a Debye hard-core phase. Also shown is the cross section due to the hard core alone and the classical hard-core cross section. Evidently, the structure is due almost entirely to the poles. The rainbow angle is given by a simple algebraic function of the pole positions. The first few computer points have been simply connected by straight lines.

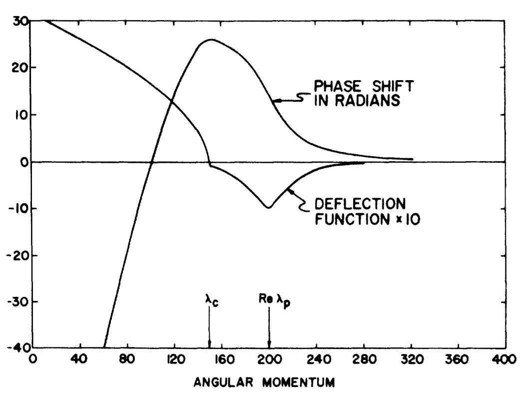


FIG. 2. The phase shift and deflection function for the configuration of 11 poles described in the text and in more detail in the caption to Fig. 3, plus a Debye hard core starting at $\lambda_C = 150$. The scattering cross section corresponding to this is given in Fig. 3.

Figure 2 contains the phase shift and deflection function which result when using these parameters. It must be emphasized that the experiment cited above was used only to suggest relevant parameter values for a numerical example. In a serious fitting attempt, modifications would be made to improve the bumpy shape of the deflection function; for present purposes it serves to enable one to distinguish clearly the basic shapes of the core and the pole by marking the boundary between the two regions.

In Fig. 3 one has the cross section averaged over an angular window of 2°. The core contribution was obtained directly by summation up to $\lambda_C = 150$. This figure shows that the characteristic oscillations observed, including the rainbow, are all basically contained in the pole contribution.

A careful analysis of such experiments along these lines might involve a least-squares fit to the data while varying $\lambda_C$ and the $\lambda_p$. This would result in a best analytic expression for the $S$ matrix in which the informational content of the experiment was conveniently codified. One could then, if desired, obtain the implied potential via the well-known WKB-based inversion formula.[15]

## IV. POLES NEAR THE REAL AXIS

Any physical phenomenon which causes large and/or rapid changes in the phase shift over finite intervals of $\lambda$ implies singularities of $S$ near the positive real axis. Below the onset of inelasticity the singularities must be simple poles[7]; above, they may be more complicated but could of course be approximated by simple poles.

Two common phenomena of this type which come to mind are orbiting[16] and level crossing.[17] In the case of orbiting one has a range of angular momenta in which there are a number of resonances. A packet composed mainly of such angular momenta will remain in the vicinity of the potential a relatively long time before dissipating; hence, its center must orbit some time about the potential center.

In the case of level crossing, particles whose trajectory remains a relatively long time in the region of crossing will be preferentially depleted from the elastic channel. The phase shift at angular momenta close to values corresponding to such trajectories must again suffer large changes in their real and imaginary parts. This may also be parametrized, without unitarity, using poles near the positive real axis.

As Eq. (17) indicates, poles near the axis will contribute both positive and negative frequency oscillations in angle to $ikf_T$. Consider the case of orbiting in which for each pole $\mathrm{Im}\lambda_P > 0$. Equation (17) may be expanded into a convergent series in powers of $e^{2\pi i\lambda_P}$, each term of which allows an interesting interpretation in terms of ray theory. The contribution $(-1)^m e^{2\pi i m\lambda} Q_{\lambda-1/2}(x-i0)$ arises from rays performing $m$ complete orbits before escaping. During each complete orbit the ray experiences a phase change $2\pi\,\mathrm{Re}\lambda_P = k\times(2\pi r_P)$ = wave number $\times$ circumference of $P$th orbit; it experiences an intensity loss $(e^{-2\pi|\mathrm{Im}\lambda_P|})^2$. From this one can deduce the approximate half-life of the resonance associated with the pole as follows: The number of revolutions to halve intensity $N$ is given by $N\,2\pi\,|\mathrm{Im}\lambda_P| = \frac{\pi}{2}$; the distance traversed in these $N$ revolutions is $2\pi N r_P = \frac{1}{2}(r_P/\mathrm{Im}\lambda_P) = (1/2k)\times(\mathrm{Re}\lambda_P/\mathrm{Im}\lambda_P)$; the time taken to go this distance is distance/velocity $= (m/2k^2)(\mathrm{Re}\lambda_P/\mathrm{Im}\lambda_P)$ = half-life.[18] The terms multiplying $Q_{\lambda-1/2}(x+i0)$ have a similar interpretation; they correspond to rays traveling in the opposite sense and which must execute at least one full orbit before escaping.

One can finally ask about the qualitative features of the contribution to the amplitude of a group of such poles. As a simple model consider a sequence of $N$ such poles equally spaced parallel to, and above, the real axis. Their main contribution to the scattering amplitude is of form [using (17) and (21)]

$$\sum_{P=1}^{N} e^{i\lambda_P\theta} = e^{i\lambda_1}\sum_{n=0}^{N-1} e^{in\Delta\theta}$$

$$= e^{i\lambda_N/2\theta}(\sin\tfrac{1}{2}N\Delta\theta)/(\sin\tfrac{1}{2}\Delta\theta)\ , \qquad (30)$$

where $\Delta = \lambda_{P+1} - \lambda_P$. This function has its first major maximum at $\theta_{\max} = 2\pi/\Delta$ with width $\sim (1/N)\theta_{\max}$. Thus, the net effect of an orbiting situation or a single level crossing will often be a few widely spaced narrow blips superimposed in the background amplitude.

## V. TOTAL CROSS SECTIONS

It is of some interest to ask, in the context of the present results, to what extent the total cross section can be inferred from partial knowledge of the differential cross section. A large contribution to the total cross section comes from small-angle scattering. Differential cross-section measurements have of necessity an associated minimum angle of measurement. Therefore, to infer the total cross section, a theoretical extrapolation must in effect be performed. Low-angle scattering is dominated by diffraction plus refractive scattering of high partial waves by the asymptotic tail of the potential. It is the latter which are not directly observed in the differential-cross-section experiment. The diffractive contribution can be inferred to within the accuracy of the differential-cross-section experiment, since it is determined by the phase shift at low and intermediate partial waves, and these phases are in turn determined by the intermediate and high-angle cross-section data.

One has from the optical theorem

$$\sigma = (4\pi/k)\,\mathrm{Im}f(0) = -(4\pi/k^2)\textstyle\sum_\lambda \lambda(S-1)\ . \qquad (31)$$

If one were to use the expression for $f$ obtained via methods presented here from a differential-cross-section analysis one would write

$$\sigma = \sigma_C + \sigma_T = (4\pi/k)\,\mathrm{Im}f_C(0) + (4\pi/k)f_T(0)\ . \qquad (32)$$

However, note that one can write

$$S_T = \textstyle\sum_P C_P(\lambda_P^2 - \lambda_P^{*2})(\lambda^2 - \lambda_P^2)^{-1} + 1\ , \qquad (33)$$

$$S_T - 1 = [\textstyle\sum_P C_P(\lambda_P^2 - \lambda_P^{*2})]\lambda^{-2} + O(\lambda^{-4})\ , \qquad (34)$$

so that unless the poles are carefully balanced to eliminate the leading term in the asymptotic expansion Eq. (34), the long-range behavior of $S-1$ is as $\lambda^{-2}$ and corresponds to an inverse power potential going as $r^{-3}$. It is most often true that the potential decreases at a faster rate, while even if it did decrease as $r^{-3}$ the coefficient of this term obtained from a fitting procedure may be incorrect due to ignorance of small-enough-angle data. One should therefore write

$$\sigma = \sigma_C + \sigma_T + \Delta\sigma_T \,, \tag{32'}$$

where

$$\Delta\sigma_T = -\frac{4\pi}{k^2}\,\mathrm{Re}\sum_{\lambda=\lambda_A}^{\infty} \lambda(S - S_T) \tag{35}$$

and $S$ is the true matrix having correct asymptotic form, while $\lambda_A$ is the lowest $\lambda$ such that

$$S(\lambda_A) - S_T(\lambda_A) \cong 0 \,, \quad \Theta(\lambda_A) - \Theta_T(\lambda_A) \cong 0 \,. \tag{36}$$

One might empirically determine $\lambda_A$ by noting that it should be near that value of $\lambda$ such that the refracted waves cross the minimum angle of resolution $\theta_{\min}$ of the experiment,

$$\Theta_T(\lambda_A) \cong \theta_{\min} \,. \tag{37}$$

One can therefore only proceed by estimating $S$ for $\lambda \geq \lambda_A$ using additional information concerning the long-range part of the interatomic potential. $\Delta\sigma$ can be then calculated; $\sigma_C$ is again probably best calculated by simply summing the series $\lambda_C$; $\sigma_T$ can be given analytically using the behavior[19] of the $Q$ functions $\theta = 0$;

$$\sigma_T = (4\pi/k^2)\,\mathrm{Re}\textstyle\sum_P C_P \big[\,|\lambda_P^2 - \lambda_P^{*2}| + (2/\pi)(\lambda_P^2 - \lambda_P^{*2})\,\psi(\lambda_P + \tfrac{1}{2})\big] \,, \tag{38}$$

$$\psi(z) = \ln z - (2z)^{-1} - O(z^{-2}) \,.$$

## ACKNOWLEDGMENTS

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[2]M. V. Berry, Proc. Phys. Soc. (London) 89, 479 (1966); F. J. Smith, E. A. Mason, and J. T. Vanderslice, J. Chem. Phys. 42, 3257 (1965).

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[8]One uses various formulas from Sec. 3.4 of *Higher Transcendental Functions*, edited by A. Erdelyi (McGraw-Hill, New York, 1953), Vol. 1. Note Eq. 3.4 (8) has a sign mistake; compare with Eq. 8.3.3 of Ref. 9.

[9]*Handbook of Mathematical Functions*, edited by M. Abramowitz and I. Stegun, Natl. Bur. Std. Applied Mathematics Series No. 55 (U. S. GPO, Washington, D. C., 1968).

[10]Reference 8, Eq. 3.5(4).

[11]Reference 8, Sec. 3.9.1. The condition that the $n$th term be less than the $(n-1\text{th})$ in magnitude is obtained directly from Eq. 21: $f_n|\zeta|^n < f_{n-1}|\zeta|^{n-1}$. This leads directly to $n < (1 + 2\lambda\sin\theta)/(1 - 2\sin\theta)$. For $\theta \ll 30°$ we see that $2\lambda\theta \gg 1$ is necessary for the existence of many decreasing terms and, hence, high accuracy. For angles $\theta \lesssim \frac{1}{2}\lambda$ one must use a small-angle approximation such as is noted in Ref. 19.

[12]Reference 9, Eq. 6.1.47.

[13]R. L. Champion, L. D. Doverspike, W. G. Rich, and S. M. Bobbio, Phys. Rev. A 2, 2327 (1970).

[14]Since such poles can strongly influence total cross section (see Sec. V) and the long-range behavior of the potential inferred from experiment, this points to an inherent ambiguity in attempting to extract the potential from the differential cross-section data.

[15]See, e.g., G. Vollmer and H. Kruger, Phys. Letters 28A, 165 (1968).

[16]In a footnote to Ref. 4, the relationship between orbiting and Regge poles was already noted in a reference to Ford and Wheeler's paper (Ref. 1).

[17]See, e.g., S. Geltman, *Topics in Atomic Collision Theory* (Academic, New York, 1969).

[18]Compare with the discussion in Ref. 7, Sec. 9.5 and also with the discussion of "surface waves" in Ref. 6.

[19]Reference 8, Eq. 3.9.2(7).