42

The Rayleigh–Faxen–Holtzmark Partial Wave Expansion: Phase Shift Method

We shall now solve the scattering problem, that is, find solutions for the Schrödinger equation [eq. (18) of Chapter 41] in the form of eq. (19) of Chapter 41 for a spherically symmetric $V(r)$ that goes to zero faster than $1/r^2$ as $r \to \infty$. [Note: For such a potential, the effective $V(r)$ approaches the pure centrifugal term for sufficiently large r. Also, we exclude for the moment the case of scattering via a Coulomb potential with a $V(r)$ that goes to zero only as $1/r$ at large r. Our assumed $V(r)$ would be good for the scattering of neutrons from complex nuclei, but the scattering of charged particles from nuclei, e.g., the scattering of protons or alpha particles from nuclei, would require a slightly more complicated treatment.]

We shall expand the solution to the relative motion equation

$$\nabla^2\psi + \frac{2\mu}{\hbar^2}(E - V(r))\psi = 0 \tag{1}$$

in a series similar to that of the expansion of the incoming plane wave of Chapter 41

$$\psi = \sum_{l=0}^{\infty} \frac{w_l(kr)}{(kr)} P_l(\cos\theta). \tag{2}$$

This equation is the partial wave expansion. The ψ are independent of the azimuth angle, ϕ. This axial symmetry is dictated by the spherical symmetry of $V(r)$ and the axial symmetry about the direction of the incoming beam. In the above, the l^{th} partial wave solution is determined by the radial function, $R_l(kr) \equiv w_l(kr)/(kr)$, which is a solution of the one-dimensionalized wave equation

$$\frac{d^2 w_l}{dr^2} + \left(k^2 - \frac{2\mu}{\hbar^2} V(r) - \frac{l(l+1)}{r^2}\right) w_l = 0. \tag{3}$$

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As $r \to \infty$, $V(r) \to 0$, such that $V_{\text{effective}} \to V_{\text{centrifugal}}$. Thus, $w_l(kr) \to$ is a linear combination of the free-wave radial solutions $(kr)j_l(kr)$ and $(kr)n_l(kr)$. From their asymptotic form [see eq. (44) of Chapter 41], this is a linear combination of $\sin(kr - \frac{l\pi}{2})$ and $\cos(kr - \frac{l\pi}{2})$, so, as $r \to \infty$,

$$\begin{aligned} w_l(kr) &\to a_l \sin(kr - \tfrac{l\pi}{2} + \delta_l(k)), \\ \frac{w_l(kr)}{(kr)} &\to \frac{a_l}{2ikr}\Big(e^{ikr}(-i)^l e^{i\delta_l} - e^{-ikr}(i)^l e^{-i\delta_l}\Big). \end{aligned} \tag{4}$$

Here, a_l is the amplitude of the l^{th} partial wave, and δ_l, an energy (k)-dependent quantity, is its phase shift. To find the differential scattering cross section, we need to compare these partial wave solutions with the expected asymptotic form of our solution

$$\psi = e^{i\vec{k}\cdot\vec{r}} + f(\theta)\frac{e^{ikr}}{r}. \tag{5}$$

Expanding, $f(\theta)$, through

$$f(\theta) = \sum_{l=0}^{\infty} f_l P_l(\cos\theta), \tag{6}$$

and using eq. (52) of the last chapter to expand the plane wave, we have, as $r \to \infty$,

$$\begin{aligned} \psi &\to \sum_l \Big(i^l(2l+1)\frac{sin(kr - \frac{\pi}{2}l)}{kr} + f_l\frac{e^{ikr}}{r}\Big)P_l(\cos\theta) \\ &\to \sum_l \Big(\frac{e^{ikr}}{r}(f_l + \frac{(2l+1)}{2ik}) - \frac{e^{-ikr}}{r}\frac{(-1)^l(2l+1)}{2ik}\Big)P_l(\cos\theta). \end{aligned} \tag{7}$$

Comparing with eqs. (2) and (4),

$$a_l = i^l(2l+1)e^{i\delta_l} \qquad \text{and} \qquad f_l = \frac{(2l+1)}{2ik}(e^{2i\delta_l} - 1), \tag{8}$$

so

$$\begin{aligned} f(\theta) &= \sum_{l=0}^{\infty}\frac{i(2l+1)}{2k}(1 - e^{2i\delta_l(k)})P_l(\cos\theta) \\ &= \sum_{l=0}^{\infty} e^{i\delta_l(k)}\frac{(2l+1)}{k}\sin\delta_l(k)P_l(\cos\theta), \end{aligned} \tag{9}$$

leading to

$$\begin{aligned} \frac{d\sigma}{d\Omega} = |f(\theta)|^2 &= |\sum_l \frac{(2l+1)}{2k}(1 - \eta_l)P_l(\cos\theta)|^2 \\ &= |\sum_l e^{i\delta_l}\frac{(2l+1)}{k}\sin\delta_l P_l(\cos\theta)|^2, \end{aligned} \tag{10}$$

where the common shorthand notation, $\eta_l = e^{2i\delta_l}$, has been used in the first form. Using the orthogonality integral

$$\int\int d\Omega P_l(\cos\theta) P_{l'}(\cos\theta) = \frac{4\pi}{(2l+1)} \delta_{ll'}, \tag{11}$$

these two expressions lead to expressions for the total cross section

$$\begin{aligned} \sigma &= \sum_l \frac{\pi}{k^2}(2l+1)|1-\eta_l|^2 \\ &= \sum_l \frac{4\pi}{k^2}(2l+1)\sin^2\delta_l. \end{aligned} \tag{12}$$

A number of remarks are in order, as follows.

1. For $V(r) \to 0, \delta_l(k) \to 0$. In this case, we are left only with the free incoming plane wave.

2. In the limit of very large k, in particular, for $\frac{\hbar^2 k^2}{2\mu} \gg |V_{\max}|$, again $\delta_l(k) \to 0$ as $k \to$ very large. Effectively, the potential again becomes insignificant compared with the energy of the incoming beam.

3. For an attractive $V(r)$, $\delta(k) > 0$. In this case, the wavelength becomes shorter in the small r region where the potential is effective, and the l^{th} partial wave is pulled into smaller values of r as a result (see Fig. 42.1). Say the first minimum of the l^{th} partial wave beyond the region where the true $V(r)$ is effectively zero occurs at a phase angle, χ_1. Then, $(kr_{\text{with}} - \frac{\pi l}{2} + \delta_l) = (kr_{\text{without}} - \frac{\pi l}{2}) = \chi_1$, where r_{with} is the position of this minimum *with* the potential $V(r)$ turned on, whereas r_{without} is the position of this minimum *without* the potential, that is, for the free partial wave. Because $r_{\text{with}} < r_{\text{without}}$, $\delta_l(k) > 0$.

Similarly, for a repulsive $V(r)$, $\delta_l(k) < 0$.

4. The total scattering cross section, σ, is related to the imaginary part of the scattering amplitude, $f(\theta = 0)$. From the second form for $f(\theta)$ and σ above,

$$\sigma(k) = \frac{4\pi}{k}\Im\big[f(\theta = 0)\big]. \tag{13}$$

This form is a special case of the so-called Optical Theorem. It also leads to the Wick inequality for the elastic scattering cross section

$$\sigma_{\text{elastic}} \leq \frac{4\pi}{k}\sqrt{\frac{d\sigma}{d\Omega}(\theta = 0)}. \tag{14}$$

Note,

$$\frac{d\sigma}{d\Omega} = \big(\Im[f(\theta)]\big)^2 + \big(\Re[f(\theta)]\big)^2.$$

5. A relation exsits between the maximum l for which $\delta_l(k)$ is appreciably different from zero and the magnitude k of the incoming wave. Thus, although our expressions for both $\frac{d\sigma}{d\Omega}$ and σ in general involve an infinite series in l, only a finite number of terms may be effective. Suppose the range of our $V(r)$ is r_0; i.e., $V(r) \approx 0$ for $r > r_0$. Classically, if a projectile particle comes in with an impact parameter, $b > r_0$, it will "miss" feeling the potential and not be scattered

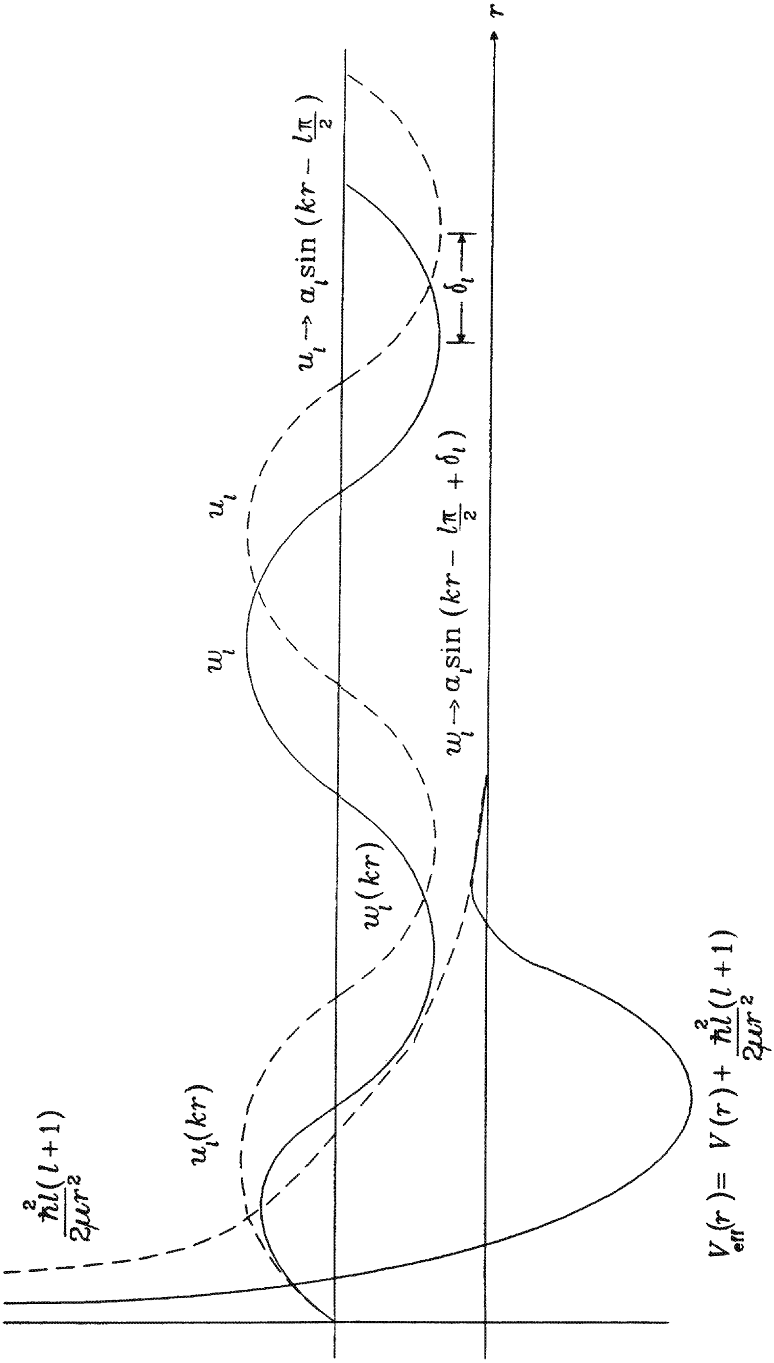

FIGURE 42.1. The lth partial wave solutions, u_l (plane wave), and w_l [with attractive $V(r)$].

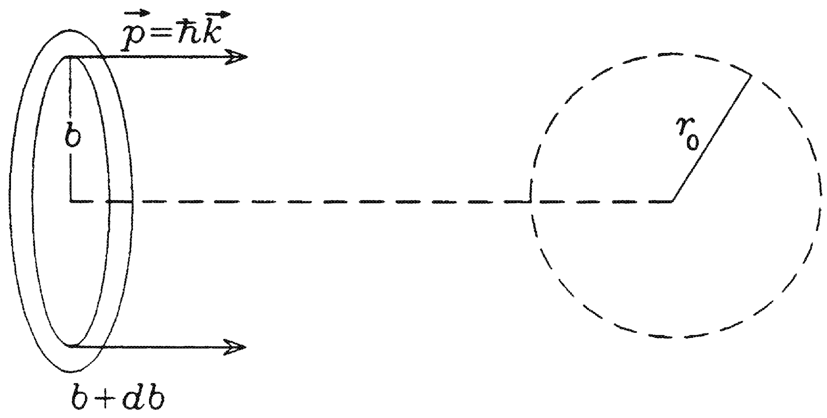

FIGURE 42.2. Semiclassical picture of the scattering process.

at all. (See Fig. 42.2.) Although the wave nature of the particle motion and the uncertainty relation washes out this relationship somewhat, it nevertheless still has approximate validity. The angular momentum of an incoming particle with impact parameter, b, is $\hbar kb$. Approximately,

$$\hbar kb \approx \hbar\sqrt{l(l+1)}, \qquad b \approx \frac{l}{k}. \tag{15}$$

Because we expect strong scattering only for $b < r_0$, we expect δ_l will be appreciably different from zero only for $l \leq kr_0$, where this relation might be a particularly good approximation for large l, where semiclassical arguments are valid. Recalling $P_l(\cos\theta) = \sqrt{4\pi/(2l+1)}Y_{l0}$, the plane wave expansion in terms of normalized angular functions, Y_{lm}, is

$$e^{ikr\cos\theta} = \sum_l i^l\sqrt{4\pi(2l+1)}j_l(kr)Y_{l0}(\theta), \tag{16}$$

so the probability of finding the l^{th} partial wave component of the plane wave within a radius r_0 is proportional to the integrated value, from 0 to r_0, of the function $(2l+1)j_l(kr)^2$. This function is plotted for the lower l values in Fig. 42.3. We see, e.g., if $kr_0 = 1.5$, only the $l = 0$ and $l = 1$ partial waves will have a large probability of penetrating into the effective range of the potential. In general, for very small k, that is, for extreme low energy scattering, only the $l = 0$ term will contribute to the differential scattering cross section. Because $P_0(\cos\theta) = 1$, independent of θ, the scattering will be isotropic. In this case,

$$f(\theta) \approx e^{i\delta_0}\frac{\sin\delta_0}{k}, \tag{17}$$

$$\frac{d\sigma}{d\Omega} = \frac{\sin^2\delta_0}{k^2}, \qquad \sigma = 4\pi\frac{\sin^2\delta_0}{k^2}. \tag{18}$$

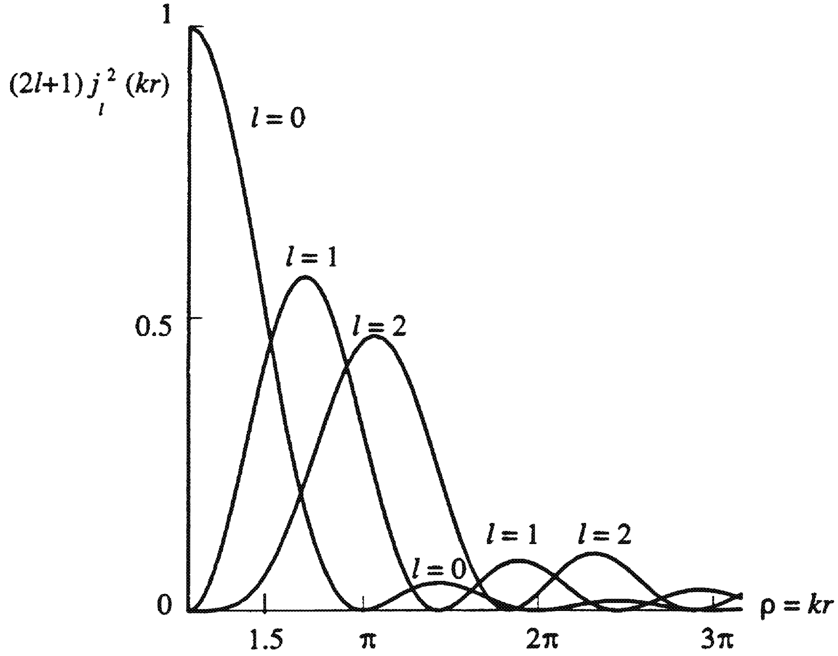

FIGURE 42.3. The functions $(2l+1)[j_l(kr)]^2$.

In the extreme low-energy limit, therefore, the cross section is proportional to the square of the wavelength. In this low-energy limit, the pertinent length is the wavelength of the incident beam, not the size of the scatterer.

If the energy is somewhat higher so both phase shifts, δ_1 and δ_0, contribute, but assuming $\delta_1 \ll 1$, then

$$\begin{aligned}\frac{d\sigma}{d\Omega} &= \frac{\sin^2\delta_0}{k^2} + \frac{6}{k^2}\cos(\delta_0 - \delta_1)\sin\delta_0\sin\delta_1\cos\theta + \cdots \\ &\simeq \frac{1}{k^2}\left(\sin^2\delta_0 + 3\delta_1\sin 2\delta_0\cos\theta + \cdots\right) \\ &= A + B\cos\theta + \cdots. \end{aligned} \tag{19}$$

With $B \ll A$, the differential cross section is almost isotropic but does now have a weak $\cos\theta$ dependence.

6. The determination of the $\delta_l(k)$ from a known $V(r)$ is in principle straightforward and just a matter of calculation. Often, however, $V(r)$ is unknown and we would like to determine it from the observed differential cross sections at different energies. Although the $\delta_l(k)$ can be determined from the observed $\frac{d\sigma}{d\Omega}$, the determination of the $V(r)$ from these $\delta_l(k)$ is difficult. The "inverse" problem is tough.

7. Generalizations to scattering of complex projectile from complex target particles. So far, we have studied only the scattering of structureless point projectile

particles from structureless point target particles. If we name projectile particle, a, and target particle, A, we have in general three possibilities, as follows.

(1) $a + A \rightarrow a + A$, the elastic scattering process.

(2) $a + A \rightarrow a + A'$. Particle A is in an excited state after the scattering process and the final kinetic energy of the relative motion is less than the initial kinetic energy. This is an inelastic scattering process.

(3) $a + A \rightarrow b + B$. This is a rearrangement collision. The ejectiles are different from the initial projectile and target particles. In such a process, the number of outgoing particles could also be greater than two.

The different processes are labeled by a "channel" index: α for the elastic process (1) and $\beta = \beta_1 + \beta_2 + \cdots$ for the processes of type (2) and (3). For the case of structureless point particles, we could have written our solution, as $r \rightarrow \infty$, in the form

$$\psi \rightarrow \sum_l \frac{i\sqrt{\pi(2l+1)v_\alpha}}{k_\alpha} i^l Y_{l0}(\theta,\phi)\Big(I_l(k_\alpha r) - \eta_{l,\alpha} O_l(k_\alpha r)\Big), \tag{20}$$

where the incoming and outgoing l^{th} partial wave relative motion functions are now given in the unit flux normalization, [see eq. (24) of Chapter 41], and

$$I_l(k_\alpha r) = \frac{1}{\sqrt{v_\alpha}} \frac{e^{-i(k_\alpha r - \frac{\pi l}{2})}}{r}, \qquad O_l(k_\alpha r) = \frac{1}{\sqrt{v_\alpha}} \frac{e^{i(k_\alpha r - \frac{\pi l}{2})}}{r}. \tag{21}$$

For the case of complex projectile and target, this process can now be generalized. Now, as $r \rightarrow \infty$,

$$\psi \rightarrow \sum_l \frac{i\sqrt{\pi(2l+1)v_\alpha}}{k_\alpha} \sum_\beta (\mathcal{I}_{l,\alpha} - \eta_{l,\beta}\mathcal{O}_{l,\beta}), \tag{22}$$

where the sum over β includes the elastic term, $\beta = \alpha$, and all other β_i, and the outgoing and incoming wave functions must now include, besides the asymptotic outgoing and incoming relative motion functions, the appropriate internal wave functions for the particles a, A, or b, and B.

$$\begin{aligned} \mathcal{I}_{l,\alpha} &= i^l Y_{l0}(\theta,\phi) I_l(k_\alpha r)\psi_{\text{internal}}(\xi_a)\psi_{\text{internal}}(\xi_A), \\ \mathcal{O}_{l,\beta} &= i^l Y_{l0}(\theta,\phi) O_l(k_\beta r)\psi_{\text{internal}}(\xi_b)\psi_{\text{internal}}(\xi_B), \end{aligned} \tag{23}$$

where the $\xi_a, \xi_A, \cdots$, stand for the needed internal variables of the various particles. Now,

$$\begin{aligned} \sigma_{\text{total}} &= \sigma_{\text{elastic}} + \sigma_{\text{reaction}} \\ &= \sigma_\alpha + \sum_{\beta \neq \alpha} \sigma_\beta \\ &= \frac{\pi}{k_\alpha^2} \sum_l \sum_{\text{all } \beta} (2l+1)|\delta_{\alpha\beta} - \eta_{l,\beta}|^2 \\ &= \frac{\pi}{k_\alpha^2} \sum_l (2l+1)\Big(|1 - \eta_{l,\alpha}|^2 + \sum_{\beta\neq\alpha} |\eta_{l,\beta}|^2\Big). \end{aligned} \tag{24}$$

Later, we shall see the conservation of probability, the so-called unitarity condition, will require

$$\Big(|\eta_{l,\alpha}|^2 + \sum_{\beta\neq\alpha} |\eta_{l,\beta}|^2\Big) = 1. \tag{25}$$

Previously, we saw for the case of pure elastic scattering, e.g., at low energies, where all inelastic processes and rearrangement collisions are energetically forbidden, $\eta_{l,\alpha} = e^{2i\delta_{l,\alpha}}$. Now, in general, $|\eta_{l,\beta}| \leq 1$. The unitarity condition severely restricts the values of the l^{th} partial cross sections, σ_l. Fig. 42.4 gives a plot of the possible values of $\sigma_{\text{elastic},l}$ versus $\sigma_{\text{reaction},l}$, both in units of $\pi(2l+1)/k_\alpha^2$.

A final remark: Eqs. (20) and (22) can also be used for the case of scattering by a Coulomb potential, provided the r dependence in the exponential factors in the incoming and outgoing relative motion functions, $I_l(kr)$ and $O_l(kr)$, are replaced by slightly more complicated r-dependent functions.

Mathematical Appendix to Chapter 42

Continuum Solutions for the Coulomb Problem

In the main body of Chapter 42, we restricted our discussion to potentials that go to zero faster than $1/r^2$ as $r \to \infty$. This, therefore, excluded the important case of the Coulomb potential, $V(r) = Z_1 Z_2 e^2/r$, needed for the scattering of point charges from point charges. We shall be interested, in particular, in the asymptotic form of the l^{th} partial wave solutions, w_l, in the limit $r \to \infty$, to obtain the analogues of the incoming and outgoing wave solutions, $I_l(kr)$ and $O_l(kr)$.

For the Coulomb potential, the one-dimensionalized wave equation is given by

$$\frac{d^2 w_l}{dr^2} + \Big(k^2 - \frac{2\mu}{\hbar^2}\frac{Z_1 Z_2 e^2}{r} - \frac{l(l+1)}{r^2}\Big) w_l = 0, \tag{1}$$

$$\frac{d^2 w_l}{dr^2} + \Big(k^2 - \frac{2\gamma k}{r} - \frac{l(l+1)}{r^2}\Big) w_l = 0, \tag{2}$$

where we have introduced the Coulomb parameter

$$\gamma = \frac{\mu e^2 Z_1 Z_2}{\hbar^2 k} = \frac{\mu c}{\hbar k}\frac{e^2}{\hbar c} Z_1 Z_2 = \frac{c}{v}\alpha Z_1 Z_2. \tag{3}$$

In addition, it will be useful to introduce the new variable

$$\rho = ikr, \tag{4}$$

so

$$-\frac{d^2 w_l}{d\rho^2} + \Big(1 - \frac{2i\gamma}{\rho} + \frac{l(l+1)}{\rho^2}\Big) w_l = 0. \tag{5}$$

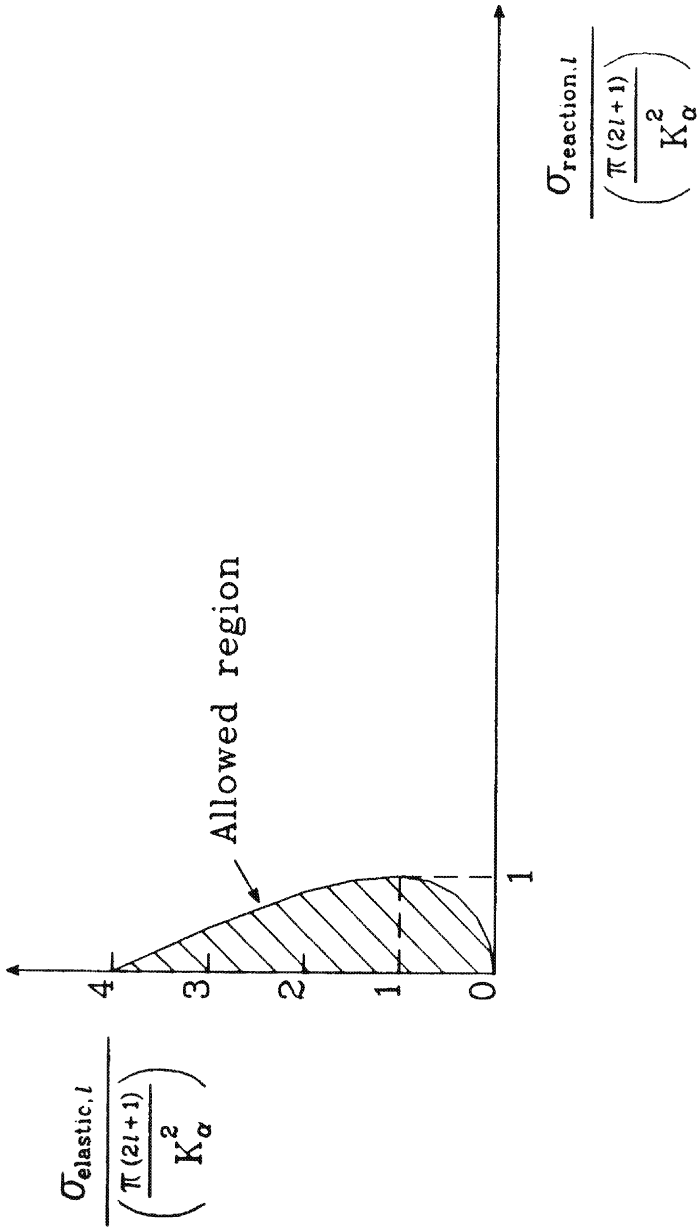

FIGURE 42.4. The domain of allowed $\sigma_{\text{elastic},l}$ vs. $\sigma_{\text{reaction},l}$.

Factoring out the asymptotic behavior of the w_l at $\rho = 0$ and $\rho = \infty$, we need solutions of the form

$$w_l = \rho^{l+1} e^{\rho} v_l(\rho), \tag{6}$$

where we restrict ourselves for the moment to the solution regular at $r = 0$ and v_l satisfies the differential equation

$$\rho v_l'' + (2l + 2 + 2\rho)v_l' + 2(l + 1 + i\gamma)v_l = 0. \tag{7}$$

With the further substitution,

$$t = -2\rho = -2ikr, \tag{8}$$

this solution can be put in the standard form

$$\begin{aligned} t\frac{d^2 v_l}{dt^2} + (2l + 2 - t)\frac{dv_l}{dt} - (l + 1 + i\gamma)v_l &= 0, \\ t v_l'' + (c - t)v_l' - a v_l &= 0, \end{aligned} \tag{9}$$

where $c \equiv (2l + 2)$ and $a \equiv (l + 1 + i\gamma)$. This is the standard form of the differential equation for the hypergeometric function of type, ${}_1F_1(a; c; t)$, the so-called confluent hypergeometric function [in a notation in which the Gaussian hypergeometric function would have been named a ${}_2F_1(a, b; c; t)$]. Substituting an infinite power series solution of the form

$$v_l = \sum_{n=0}^{\infty} c_n t^n, \tag{10}$$

we are led to a two-term recursion formula for the c_n,

$$\frac{c_n}{c_{n-1}} = \frac{(a + n - 1)}{n(c + n - 1)}, \tag{11}$$

which, with the choice $c_0 = 1$, leads to

$$c_n = \frac{a(a+1)\cdots(a+n-1)}{n!c(c+1)\cdots(c+n-1)} = \frac{(a)_n}{n!(c)_n} = \frac{\Gamma(a+n)}{n!\Gamma(a)} \frac{\Gamma(c)}{\Gamma(c+n)}, \tag{12}$$

where the c_n have been expressed in terms of Γ functions. Note, $\Gamma(a + 1) = a\Gamma(a)$ and, for the integer $c = (2l + 2)$, $\Gamma(2l + 2) = (2l + 1)!$. We then have

$$w_l(kr) = (ikr)^{l+1}(e^{ikr})\ {}_1F_1(a; c; -2ikr), \quad \text{with } a = (l+1+i\gamma), \quad c = (2l+2). \tag{13}$$

For our purposes, it will be useful to express the confluent hypergeometric function in terms of a contour integral

$${}_1F_1(a; c; t) = \frac{\Gamma(c)}{2\pi i}\oint_C \frac{dz e^z}{z^{c-a}(z - t)^a} = \frac{\Gamma(c)}{2\pi i}\oint_C \frac{dz e^z}{z^c\left(1 - \frac{t}{z}\right)^a}, \tag{14}$$

where the contour, C, in the complex z plane surrounds the branch cut from $z = 0$ to $z = t$, where the complex number t is $t = -2ikr$ in our case. The contour will be chosen such that $|\frac{t}{z}| < 1$, so we can make the expansion, which will be used to establish eq. (13),

$$ {}_1F_1(a;c;t) = \frac{\Gamma(c)}{2\pi i}\sum_{n=0}^{\infty}\frac{(a)_n}{n!}t^n \oint_C \frac{dz e^z}{z^{c+n}} = \Gamma(c)\sum_{n=0}^{\infty}\frac{(a)_n}{n!}\frac{t^n}{(c+n-1)!}, \tag{15} $$

where we have evaluated the contour integral by the residue theorem, bearing in mind $c = (2l+2)$ is an integer. Using $(a)_n = \Gamma(a+n)/\Gamma(a)$ for the complex number, a, and $(c+n-1)! = \Gamma(c+n)$ for the integer, $c+n$, we get

$$ {}_1F_1(a;c;t) = \sum_{n=0}^{\infty}\frac{\Gamma(a+n)}{\Gamma(a)}\frac{\Gamma(c)}{\Gamma(c+n)}\frac{t^n}{n!}, \tag{16} $$

which establishes the contour integral form for ${}_1F_1(a;c;t)$. It will now be useful to deform the contour C, as shown in Fig. 42.5, where the new deformed contour integral can effectively be decomposed into the two loop integrals over contours C_1 and C_2,

$$ {}_1F_1(a;c;-2ikr) = \frac{\Gamma(c)}{2\pi i}\sum_{n=1,2}\oint_{C_n}\frac{dz e^z}{z^c\left(1+\frac{2ikr}{z}\right)^a}. \tag{17} $$

If we further make the substitution, $z = krz'$, so

$$ {}_1F_1(a;c;-2ikr) = \frac{\Gamma(c)}{2\pi i(kr)^{c-1}}\sum_{n=1,2}\int_{C_n}\frac{dz' e^{krz'}}{z'^c\left(1+\frac{2i}{z'}\right)^a}, \tag{18} $$

in the new contour integrals, C_1 and C_2 (see the final form of these contours in Fig. 42.5), only the circular parts of the new contours about the points $z' = 0$ and $z' = -2i$ contribute to the contour integrals in the limit $kr \to \infty$, because the real part of z' is negative on the straight-line portions of the final forms of C_1 and C_2, so $e^{krz'} \to 0$ as $r \to \infty$. Now, to do the contour integrals for the circular parts of the contours C_1 and C_2, surrounding the points $z' = 0$ and $z' = -2i$, in the limit $kr \to \infty$, let us rename $krz' = z$, so for the first integral, for the contour C_1, we have

$$ \begin{aligned} I_1 &= \frac{\Gamma(c)}{2\pi i}\lim_{r\to\infty}\oint_{C_1}\frac{dz e^z}{z^c\left(1+\frac{2ikr}{z}\right)^a} \\ &= \frac{\Gamma(c)}{2\pi i}\lim_{r\to\infty}\frac{1}{(2ikr)^a}\oint_{C_1}\frac{dz e^z}{z^{c-a}\left(1-\frac{iz}{2kr}\right)^a} \\ &= \frac{\Gamma(c)}{2\pi i}\frac{1}{(2ikr)^a}\oint_{C_1}\frac{dz e^z}{z^{c-a}} = \frac{\Gamma(c)}{(2ikr)^a\Gamma(c-a)}, \end{aligned} \tag{19} $$

where we have replaced the contour, C_1, by a small circle around the point $z = 0$ and we have used

$$ \frac{1}{2\pi i}\oint\frac{dz e^z}{z^{c-a}} = \frac{1}{\Gamma(c-a)}. \tag{20} $$

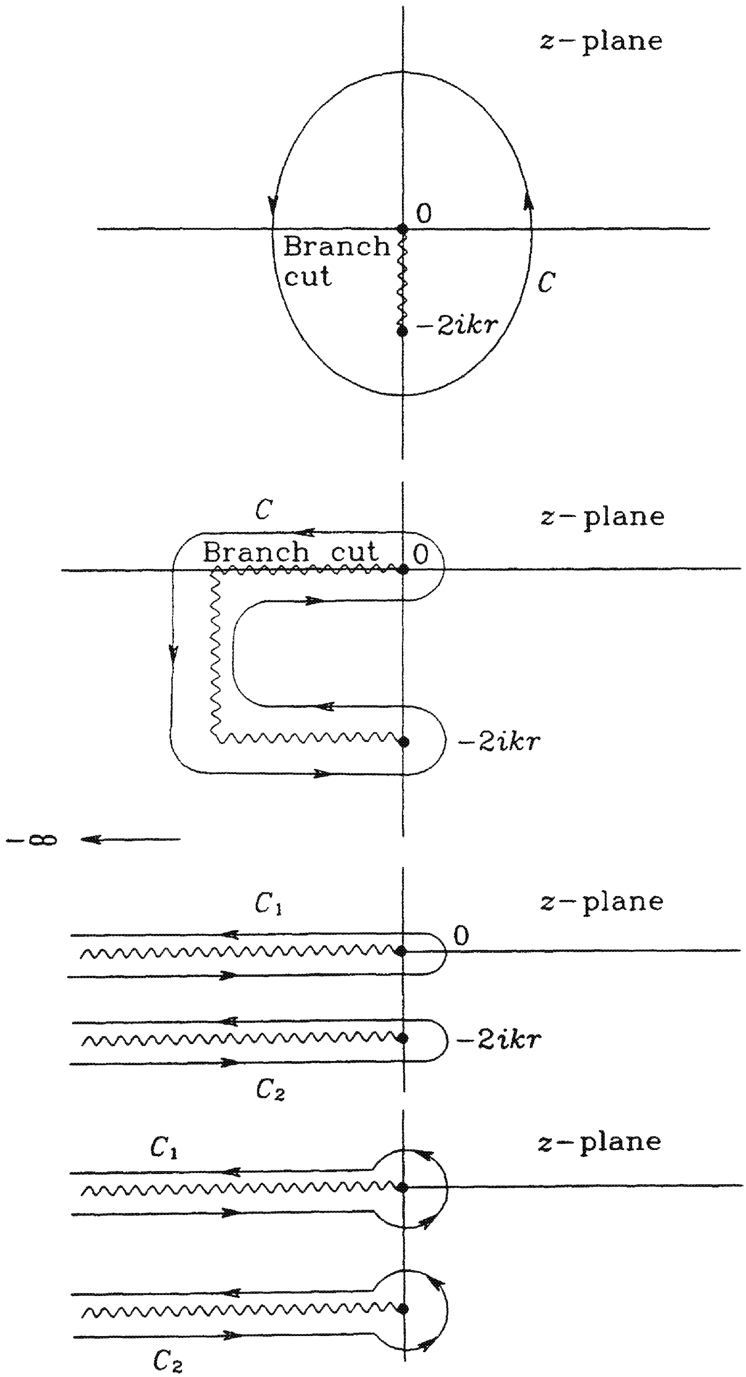

FIGURE 42.5. Contour integral for the confluent hypergeometric function and the deformed contours used to evaluate the integral.

Substituting for $c = (2l + 2)$, and $a = (l + 1 + i\gamma)$, we have, in the limit $r \to \infty$,

$$I_1 = \frac{(2l + 1)!}{\Gamma(l + 1 - i\gamma)} \frac{1}{(2ikr)^{l+1+i\gamma}}. \tag{21}$$

Similarly,

$$\begin{aligned} I_2 &= \frac{\Gamma(c)}{2\pi i} \lim_{r\to\infty} \oint_{C_2} \frac{dze^z}{z^{c-a}(z + 2ikr)^a} \\ &= e^{-2ikr} \frac{\Gamma(c)}{2\pi i} \oint_{C_2} \frac{d(z + 2ikr)e^{(z+2ikr)}}{(z + 2ikr - 2ikr)^{c-a}(z + 2ikr)^a} \\ &= \lim_{r\to\infty} \frac{e^{-2ikr}}{(-2ikr)^{c-a}} \frac{\Gamma(c)}{2\pi i} \oint_{C_2} \frac{dze^z}{z^a\left(1 - \frac{z}{2ikr}\right)^{c-a}} \\ &= \frac{e^{-2ikr}}{(-2ikr)^{c-a}} \frac{\Gamma(c)}{2\pi i} \oint_{C_2} \frac{dze^z}{z^a} = \frac{e^{-2ikr}}{(-2ikr)^{c-a}} \frac{\Gamma(c)}{\Gamma(a)}. \end{aligned} \tag{22}$$

Now, the contour, C_2, is a small circle around the point $z = -2ikr$ in the first line of this equation. This contour has then been transformed into a small circle about the point $z = 0$ in subsequent lines of this equation. Therefore, in the limit $r \to \infty$, this second contour integral gives

$$I_2 = \frac{e^{-2ikr}}{(-2ikr)^{l+1-i\gamma}} \frac{(2l + 1)!}{\Gamma(l + 1 + i\gamma)}. \tag{23}$$

Thus, we have for the solution, regular at the origin,

$$\begin{aligned} \lim_{r\to\infty} w_l &= \lim_{r\to\infty} (ikr)^{l+1}(e^{ikr}) \; {}_1F_1((l + 1 + i\gamma); (2l + 2); -2ikr) \\ &= \frac{(2l + 1)!e^{\frac{\gamma\pi}{2}}}{2^{l+1}} \left(\frac{e^{ikr}}{(2kr)^{i\gamma}\Gamma(l + 1 - i\gamma)} + \frac{(-1)^{l+1}e^{-ikr}}{(2kr)^{-i\gamma}\Gamma(l + 1 + i\gamma)} \right) \\ &= \frac{i^l(2l + 1)!e^{\frac{\gamma\pi}{2}}}{2^{l+1}|\Gamma(l + 1 + i\gamma)|} \left(e^{i(kr - \frac{\pi}{2}l - \gamma ln(2kr) + \sigma_l)} - e^{-i(kr - \frac{\pi}{2}l - \gamma ln(2kr) + \sigma_l)} \right). \end{aligned} \tag{24}$$

In the last step, we have used

$$\frac{1}{(2kr)^{\pm i\gamma}} = e^{\mp i\gamma ln(2kr)}, \tag{25}$$

and

$$\Gamma(l + 1 \pm i\gamma) = |\Gamma(l + 1 + i\gamma)|e^{\pm i\sigma_l}, \tag{26}$$

where σ_l is the argument of the complex number $\Gamma(l + 1 + i\gamma)$. (σ_l is a fairly standard mathematical notation for this quantity, not to be confused with a partial cross section!). Except for an overall constant

$$\frac{i^l(2l + 1)!e^{\frac{\gamma\pi}{2}}}{2^l|\Gamma(l + 1 + i\gamma)|},$$

as $r \to \infty$,

$$R_l(kr) = \frac{w_l(kr)}{ikr} \to \frac{\sin\left(kr - \frac{\pi}{2}l - \gamma ln(2kr) + \sigma_l\right)}{kr}, \tag{27}$$

which, in the limit in which the Coulomb parameter, γ, can be set equal to zero, is the asymptotic form of $j_l(kr)$.

If we define a $w_l^{(1)}(kr)$ and a $w_l^{(2)}(kr)$, such that

$$\begin{aligned}\frac{(w_l^{(1)}-w_l^{(2)})}{(ikr)} &= (ikr)^l(e^{ikr})\ {}_1F_1((l+1+i\gamma);(2l+2);-2ikr)\\ &= \frac{i^l(2l+1)!e^{\frac{\gamma\pi}{2}}}{2^l|\Gamma(l+1+i\gamma)|}\frac{F_l(kr)}{kr},\end{aligned} \tag{28}$$

the Coulomb function, $F_l(kr)/(kr)$, is the analogue of $j_l(kr)$, with

$$\lim_{r\to\infty} F_l(kr) = \sin\big(kr - \tfrac{1}{2}\pi l - \gamma ln(2kr) + \sigma_l\big). \tag{29}$$

Similarly, the linear combination

$$\frac{(w_l^{(1)}+w_l^{(2)})}{(kr)} = -\frac{i^l(2l+1)!e^{\frac{\gamma\pi}{2}}}{2^{l+1}|\Gamma(l+1+i\gamma)|}\frac{G_l(kr)}{kr}, \tag{30}$$

where the Coulomb function, $G_l(kr)/(kr)$, is the analogue of $-n_l(kr)$, with

$$\lim_{r\to\infty} G_l(kr) = \cos\big(kr - \tfrac{1}{2}\pi l - \gamma ln(2kr) + \sigma_l\big). \tag{31}$$

[The $w_l^{(1)}$ and $w_l^{(2)}$ are the generalizations of the spherical Hänkel functions, $h_l^{(1)}$ and $h_l^{(2)}$.]

For Coulomb scattering, therefore, the generalizations of the outgoing and incoming waves of eq. (21), are

$$\begin{pmatrix} O_l^{\text{Coul.}}(kr) \\ I_l^{\text{Coul.}}(kr)\end{pmatrix} = \frac{(G_l(kr) \pm i F_l(kr))}{r\sqrt{v}}, \tag{32}$$

with asymptotic form

$$\lim_{r\to\infty}\begin{pmatrix} O_l^{\text{Coul.}}(kr) \\ I_l^{\text{Coul.}}(kr)\end{pmatrix} = \frac{e^{\pm i(kr-\frac{1}{2}\pi l-\gamma ln(2kr)+\sigma_l)}}{r\sqrt{v}}. \tag{33}$$

It will also be important to give the radial Coulomb functions, regular at the origin, the proper normalization to make these part of a complete orthonormal set. For this purpose, it is sufficient to compare the asymptotic limits, as $r \to \infty$, of the plane wave solutions with the Coulomb functions in the high-energy limit in which the Coulomb parameter $\gamma \to 0$. Because we will use both Dirac delta function and box normalizations, we shall use $\mathcal{N}e^{i\vec{k}\cdot\vec{r}}$ for the plane wave solution, with $\mathcal{N} = (1/2\pi)^{\frac{3}{2}}$, or $\mathcal{N} = (1/\sqrt{\text{Vol.}})$. The partial wave expansion is

$$\begin{aligned}\mathcal{N}e^{i\vec{k}\cdot\vec{r}} &= \mathcal{N}\sum_l i^l(2l+1)j_l(kr)P_l(\cos\Theta)\\ &= \mathcal{N}4\pi\sum_{l,m} i^l j_l(kr)Y^*_{lm}(\theta_k,\phi_k)Y_{lm}(\theta,\phi)\\ &\to \mathcal{N}4\pi\sum_{l,m} i^l\left[\frac{e^{i(kr-\frac{l\pi}{2})}-e^{-i(kr-\frac{l\pi}{2})}}{2ikr}\right]Y^*_{lm}(\theta_k,\phi_k)Y_{lm}(\theta,\phi),\end{aligned} \tag{34}$$

where Θ is the angle between the vectors $\vec{r}$ and $\vec{k}$, and θ, ϕ are the polar and azimuth angles of the vector $\vec{r}$, and θ_k, ϕ_k are those of $\vec{k}$. This solution is to be compared with the partial wave expansion of the continuum Coulomb wave function

$$\begin{aligned}\psi_{\text{Coul.}}(r,\theta,\phi) &= \sum_{l,m} R_l(kr) Y_{lm}(\theta,\phi)\\ &= \sum_{l,m} A_{lm}(ikr)^l e^{ikr}[{}_1F_1((l+1+i\gamma);(2l+2);-2ikr)]Y_{lm}(\theta,\phi)\\ &\to \sum_{l,m} A_{lm}\frac{i^l(2l+1)!e^{\frac{\gamma\pi}{2}}}{2^l|\Gamma(l+1+i\gamma)|}\\ &\times\left[\frac{e^{i(kr-\frac{\pi}{2}l-\gamma ln(2kr)+\sigma_l)}-e^{-i(kr-\frac{\pi}{2}l-\gamma ln(2kr)+\sigma_l)}}{2ikr}\right]Y_{lm}(\theta,\phi). \end{aligned} \tag{35}$$

Comparing these expressions, we see that

$$A_{lm} = \mathcal{N}|\Gamma(l+1+i\gamma)|e^{-\frac{\gamma\pi}{2}}\frac{2^l}{(2l+1)!}4\pi Y^*_{lm}(\theta_k,\phi_k), \tag{36}$$

so

$$\begin{aligned}\psi_{\text{Coul.}}(r,\theta,\phi) &= \sum_{l,m}\mathcal{N}|\Gamma(l+1+i\gamma)|e^{-\frac{\gamma\pi}{2}}2^l 4\pi Y^*_{lm}(\theta_k,\phi_k)(ikr)^l e^{ikr}\\ &\times\frac{1}{2\pi i}\oint_C\frac{dz e^z}{z^{l+1-i\gamma}(z+2ikr)^{l+1+i\gamma}}Y_{lm}(\theta,\phi).\end{aligned} \tag{37}$$

In this expansion, $|\Gamma(l+1+i\gamma)|$ can be related to $|\Gamma(1+i\gamma)|$ via repeated use of the relation $\Gamma(1+z) = z\Gamma(z)$, and

$$|\Gamma(1+i\gamma)|^2 = i\gamma\Gamma(i\gamma)\Gamma(1-i\gamma) = \frac{\pi\gamma}{\sinh\pi\gamma}. \tag{38}$$

Here, the product of Γ functions has been expressed in terms of a beta function, B,

$$\begin{aligned}\Gamma(i\gamma)\Gamma(1-i\gamma) = \Gamma(1)B(i\gamma,1-i\gamma) &= 2\int_0^{\pi/2} d\theta\cos^{2i\gamma-1}\theta\sin^{1-2i\gamma}\theta\\ &= 2\int_0^{\infty}\frac{ds s^{2i\gamma-1}}{(s^2+1)}.\end{aligned} \tag{39}$$

The s integral can be done by contour integration techniques.

An Application: Electric Dipole Moment Matrix Element Between the Hydrogen Ground State and a Continuum State

For the photoelectric effect in the hydrogen atom (to be discussed in detail in Chapter 64), we shall need the matrix element of the electric dipole operator, $e\vec{r}$, between the hydrogen atom ground state, $|n=1,l=0,m=0\rangle$, and a continuum state in which the electron is ejected with momentum, $\hbar\vec{k}$, in a direction given by angles, θ_k, ϕ_k, with respect to a laboratory-fixed unit vector, $\vec{e}$; i.e., we shall need the matrix element

$$\langle \vec{k} | (\vec{r} \cdot \vec{e}) | n = 1, l = 0, m = 0 \rangle.$$

If we choose $\vec{e}$ to lie in the laboratory z direction, only the $l = 1, m = 0$ term in the partial wave decomposition of eq. (37) can make a contribution to the matrix element. Also, with $Z_1 = -1$ (electron) and $Z_2 = +1$ (proton), the Coulomb parameter, γ, is negative. It will therefore be convenient to change notation and let γ stand for the absolute value of the Coulomb parameter, [requiring a change of sign in eq. (37)]. Then,

$$\begin{aligned}
&\langle \vec{k} | (\vec{r} \cdot \vec{e}_z) | n = 1, l = 0, m = 0 \rangle \\
&= \mathcal{N} |\Gamma(2 - i\gamma)| e^{+\frac{\gamma\pi}{2}} 2(4\pi) Y^*_{10}(\theta_k, \phi_k) \int d\Omega Y^*_{10}(\theta, \phi) \cos\theta Y_{00}(\theta, \phi) \\
&\times \int_0^\infty dr r^3 e^{ikr} (ikr) \frac{2e^{-(r/a_0)}}{a_0^{\frac{3}{2}}} \frac{1}{2\pi i} \oint \frac{dz e^z}{z^{2+i\gamma}(z + 2ikr)^{2-i\gamma}} \\
&= \mathcal{N} |\Gamma(2 - i\gamma)| e^{+\frac{\gamma\pi}{2}} 2\sqrt{(4\pi)} \cos\theta_k \int_0^\infty dr r^3 e^{ikr} (ikr) \frac{2e^{-(r/a_0)}}{a_0^{\frac{3}{2}}} \\
&\times \frac{1}{2\pi i} \oint \frac{dz e^z}{z^{2+i\gamma}(z + 2ikr)^{2-i\gamma}},
\end{aligned} \tag{40}$$

where a_0 is the Bohr radius. It will be convenient to make the transformation, $z = 2ikr(z' - \frac{1}{2})$, in the contour integral and the transformation, $r = a_0 r'$, in the radial integral. Performing the radial integral first

$$\int_0^\infty dr' r' e^{-r'} e^{2ika_0 r' z'} = \frac{1}{(1 - 2ika_0 z')^2}, \tag{41}$$

and using the identity

$$ka_0 = \frac{1}{\gamma},$$

the matrix element of $(\vec{r} \cdot \vec{e}_z)$ becomes

$$\frac{\mathcal{N} |\Gamma(2 - i\gamma)| e^{\frac{\gamma\pi}{2}} \sqrt{4\pi} \cos\theta_k \gamma^4 a_0^{\frac{5}{2}}}{8} \frac{1}{2\pi i} \oint_C \frac{dz'}{(z' - \frac{1}{2})^{2+i\gamma}(z' + \frac{1}{2})^{2-i\gamma}(z' + \frac{i\gamma}{2})^2},$$

where the transformation $z = 2ikr(z' - \frac{1}{2})$ has transformed the counterclockwise contour C around the branch cut between $z = 0$ and $z = -2ikr$ in the z plane (see Fig. 42.5) into a counterclockwise contour around the branch cut between $z' = -\frac{1}{2}$ and $z' = +\frac{1}{2}$ in the z' plane (see Fig. 42.6). Besides this branch cut, there is now a singular point at $z' = -\frac{1}{2} i\gamma$. The integrand vanishes for large values of $|z'|$; and the contour C can be transformed into a clockwise contour, C', around the singular point at $z' = -\frac{1}{2} i\gamma$. Residue theory shows this contour integral has the value

$$-\frac{d}{dz'} \Big[(z' - \tfrac{1}{2})^{-2-i\gamma} (z' + \tfrac{1}{2})^{-2+i\gamma} \Big] \Big|_{z' = -(i\gamma)/2} = \left(\frac{\gamma + i}{\gamma - i} \right)^{i\gamma} \frac{64 i\gamma}{(\gamma^2 + 1)^3}$$

$$= e^{-2\gamma \tan^{-1}(1/\gamma)} \frac{64 i \gamma}{(\gamma^2+1)^3}. \tag{42}$$

Also, using eq. (38), and

$$|\Gamma(2-i\gamma)|^2 = (\gamma^2+1)|\Gamma(1-i\gamma)|^2, \tag{43}$$

we get

$$\langle \vec{k}|\vec{r}\cdot\vec{e}_z|n=1, l=0, m=0\rangle =$$
$$\mathcal{N}\sqrt{4\pi}\cos\theta_k \left[\frac{(\gamma^2+1)\pi\gamma}{\sinh \pi\gamma}\right]^{\frac{1}{2}} e^{\frac{\gamma\pi}{2}} a_0^{\frac{5}{2}} \frac{8 i \gamma^5}{(\gamma^2+1)^3} e^{-2\gamma \tan^{-1}(1/\gamma)}. \tag{44}$$

The square of the absolute value of this matrix element can be put into the following convenient form

$$|\langle \vec{k}|(\vec{r}\cdot\vec{e}_z)|100\rangle|^2 = 512\pi^2\cos^2\theta_k a_0^5 \mathcal{N}^2 \frac{\gamma^{11}}{(\gamma^2+1)^5} \frac{e^{-4\gamma \tan^{-1}(1/\gamma)}}{(1-e^{-2\gamma\pi})}. \tag{45}$$

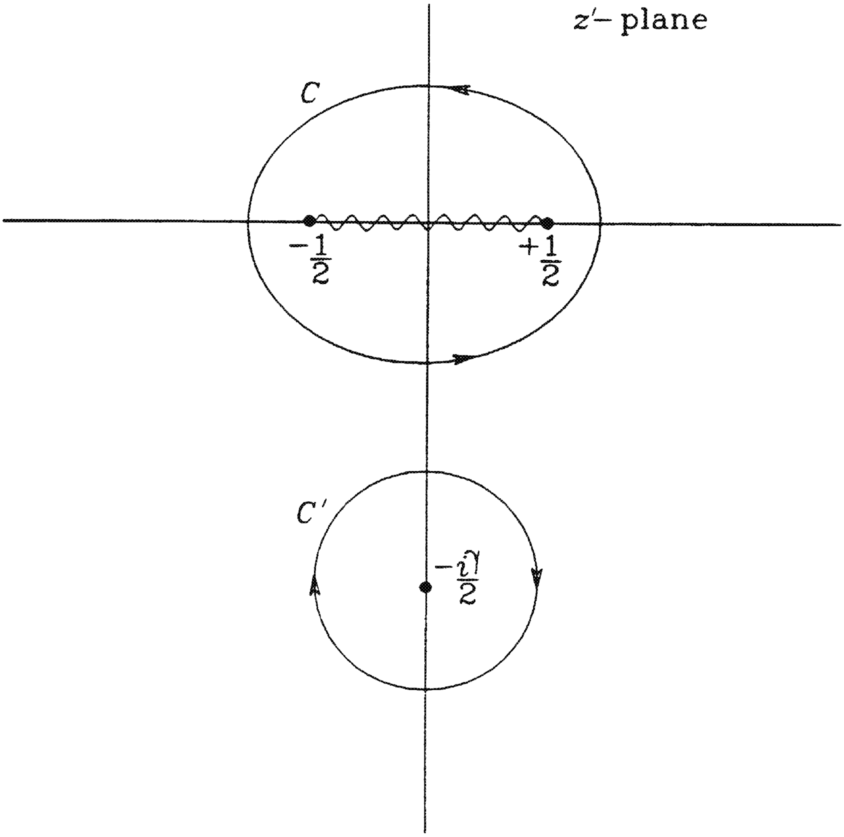

FIGURE 42.6. The z' plane contour integral.