

Semiclassical Description of Scattering

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The quantum-mechanical scattering amplitude can be simply related to the classical deflection function when the conditions for a semiclassical analysis of the quantum-mechanical scattering are met. Various interesting characteristic features of the scattering are related to special features of the classical deflection function. The characteristic types of scattering discussed are: interference, when the deflection function possesses more than one branch at a given angle; rainbow scattering, when the deflection function has a relative maximum or minimum; glory scattering, when the deflection function passes smoothly through 0° or through an integral multiple of $\pm\pi$; and orbiting, when the deflection function possesses a singularity. The consideration of the characteristic features of semiclassical scattering makes possible the analysis of an observed differential cross section to yield the classical deflection function, which in turn may be used to construct the potential.

I. INTRODUCTION

The approach of quantum-theoretical results to the results of classical theory is well understood for stationary bound states, especially through the fully-developed theory of the JWKB approximation. For continuous eigenvalues and scattering processes, the correspondence theory has been developed less thoroughly. The aim of the present paper is to focus attention on some special and interesting features of quantum scattering cross sections which appear when the scattering process may be described semiclassically.

The cross-section in the semiclassical approximation may be equal to, or very different from, the classical cross section, depending on the shape of the poten-

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tial, the bombarding energy, and the angle of observation. Although we do not discuss in detail the rate of approach of the quantum results to the classical results, it will be clear that this rate of approach is very different for different potentials, or for different angles of scattering from a given potential. The quantum and classical values for the cross section agree exactly for a Coulomb potential. However, for many potentials the quantum value converges nonuniformly to the classical cross section: for any wavelength, no matter how small, there will be an angle where quantum and classical cross sections differ by a large amount.

The semiclassical analysis of scattering not only illuminates the correspondence principle, but also may be of practical value in analysis of some nuclear and atomic scattering processes. In particular, it may provide a way to gain qualitative understanding of the results of detailed numerical calculations on the optical model of the nucleus, or to survey quickly the probable results of parameter variations.

Two of the special scattering phenomena we discuss—rainbow scattering and the glory effect—have apparently not been considered before as special features of quantum-mechanical scattering. However, these effects are well known in optics, especially in observations on the scattering of light by water droplets. In particular Van der Hulst (1)¹ has analyzed the scattering of light by spheres of homogeneous material. He has classified the simple limiting cases according as the wavelength is large or small compared to the radius of the sphere, according as the refractive index differs much or little from unity, and according as the angle of observation is small or large. He has traced out in detail the correspondence between the predictions of physical optics—as represented by the Mie-Debye scattering formula—and geometrical optics in the appropriate limiting cases, and has given formulas to cover almost all of the other limiting cases. A detailed theory of small-angle scattering has also been given by Brillouin (2).

¹ Regarding the special case of rainbow angle scattering by dielectric spheres, Van der Hulst follows the correspondence connection between geometrical optics and the Mie-Debye theory only far enough to show that classical and singular variation of intensity near a rainbow angle which corresponds to Eq. (19) below. It would be a simple matter to go to the next approximation as in Eq. (25) below and determine the diffraction pattern near a rainbow angle as an analytic function of angle. This undertaking would be all the more interesting in that there now exist for comparison detailed electronic calculations of the coefficients in the Legendre analysis of the scattered intensity, in some cases going out to harmonics of order $l = 400$: see Lowan *et al.* (1) and Gumprecht and Sliepevich (1). It is reasonable to believe that the Van der Hulst analysis, supplemented by the addition of Eq. (25) (or Eqs. 23 and 15), would allow one to obtain fairly directly and accurately the angular distribution of light scattered by transparent spheres large compared to a wavelength, in which limit the direct summation over spherical harmonics becomes more and more cumbersome. Of course this is the limit in which Airy (1) made his classic analysis of the diffraction near a rainbow angle. Further analysis of the physical optics of rainbow angle scattering appears in Pernter and Exner (1), giving additional incentive to tracing out all the yet unformulated correspondence principle relationships.

An equally full correspondence-theory analysis of the scattering of material particles has not been attempted, and is indeed much more difficult. Mott and Massey² summarize analyses to date of several of the important limiting cases and relations: resonance scattering, Born approximation scattering, and the Bohr-Peierls-Placzek conservation relations. Especially they prove that the quantum formula for the differential cross section goes over into the classical formula in the appropriate limit (discussed below). Williams (4) gives a more detailed discussion of scattering from the correspondence point of view.

II. SEMICLASSICAL APPROXIMATION AND ROLE OF CLASSICAL DEFLECTION FUNCTION

Consider the ordinary nonrelativistic scattering of a particle of reduced mass m and reduced wavelength $\lambda = \hbar/mv$ by a central potential, $V(r)$. Then the quantum expression for the differential cross section for scattering into a unit solid angle at θ has the form

$$\sigma_{qu} = |f(\theta)|^2, \quad (1)$$

where the scattering amplitude, $f(\theta)$, is given by the Rayleigh-Faxen-Holtsmark formula,

$$f(\theta) = (\lambda/2i) \sum_{l=0}^{\infty} (2l+1)(e^{2i\eta_l} - 1) P_l(\cos \theta), \quad (2)$$

in which η_l is the phase shift for the l th partial wave. The semiclassical approximation may be considered to be defined by a set of mathematical approximations introduced into (2). As the minimum set of such approximations we take the following three:

1. The phase shift η_l is replaced by its JWKB-approximate value,

$$\eta_l = \frac{1}{4}\pi + \frac{1}{2}l\pi - kr_0 + \int_{r_0}^{\infty} (k_r - k) dr, \quad (3)$$

where $k = \lambda^{-1}$, $k_r = [2M\hbar^{-2}(E - V) - (l + \frac{1}{2})^2 r^{-2}]^{1/2}$, and r_0 is the turning point of the classical motion, defined by $k_r = 0$. [In the centrifugal potential term, $l(l+1)$ is replaced by $(l + \frac{1}{2})^2$ to obtain increased accuracy (5)]. This approximation requires for its validity the physical condition of a slowly varying potential:

$$\frac{\lambda}{V} \frac{dV}{dr} \ll 1.$$

For understanding the relation between quantum and classical results, the most

² See Ref. 3. Chapter II: standard partial wave decomposition of scattering. Chapter VII, Sections 4, 5, and 6: passage to classical limit in case of very many phase shifts large compared to a radian and a monotone relation between classical deflection angle and impact parameter.

important property of the JWKB phase shift is its simple relation to the classical deflection function, $\Theta(l)$:

$$\Theta(l) = 2d\eta_l/dl. \quad (4)$$

2. The Legendre polynomial is replaced by the asymptotic expression valid for large l :

A. $\sin \theta \gtrsim 1/l$,

$$P_l(\cos \theta) \cong [1/2(l + 1/2)\pi \sin \theta]^{-1/2} \sin[(l + 1/2)\theta + \pi/4]; \quad (5)$$

B. $\sin \theta \lesssim 1/l$,

$$P_l(\cos \theta) \cong (\cos \theta)^l J_0[(l + 1/2)\theta]. \quad (6)$$

These formulas overlap slightly, so that the whole range of θ is covered. Approximation (2) requires for its validity that many l -values contribute to the scattering at a given angle or that the major contribution comes from l -values large compared to unity. However, it should be noted that formulas (5) and (6) are good approximations even at rather small l .

3. The summation of scattering amplitudes in Eq. (2) is replaced by an integral, $\Sigma_l \rightarrow \int dl$. This approximation requires for its validity that many partial waves should contribute to the scattering and that the phase shift should vary slowly and smoothly with l . It is to be noted that the possibility of making this approximation depends on defining η_l and P_l as smooth continuous functions of l , and therefore rests on approximations 1 and 2 above.

If we consider angles not too close to 0 or π , approximations 1, 2A, and 3 convert the scattering amplitude into the semiclassical form,

$$f_{sc} = -\lambda(2\pi \sin \theta)^{1/2} \int_0^\infty \left(l + \frac{1}{2}\right)^{1/2} [\exp(i\varphi_+) - \exp(i\varphi_-)] dl, \quad (7)$$

where the phases, φ_+ and φ_- , are defined by the formula

$$\varphi_\pm = 2\eta_l \pm (l + 1/2)\theta \pm \pi/4, \quad (8)$$

and the sum $\Sigma(2l + 1)P_l$ has been set equal to zero (see Ref. 3).

The three approximations just listed—use of JWKB phase shifts, use of an asymptotic formula for the Legendre polynomials, and replacement of summation by integration—together define the semiclassical treatment of scattering. However, it is often necessary to introduce a fourth approximation:

4. The integral for the scattering amplitude is evaluated by the method of stationary phase, or by the method of steepest descent, or by some other approximate method. For the result of this calculation we shall still use the descriptive phrase, “semiclassical” differential cross section,

$$\sigma_{sc} = |f_{sc}(\theta)|^2. \quad (9)$$

Applying exactly these methods, and evaluating the scattering amplitude integral by the method of stationary phase, Mott and Massey obtain the result, $\sigma_{sc} = \sigma_{cl}$, where σ_{cl} , the classical differential scattering cross section, is given by the formula,

$$\begin{aligned}\sigma_{cl} &= \lambda^2(l_\theta + \frac{1}{2}) / [\sin \theta | d\Theta/dl |_{\theta=\theta}] \\ &= \lambda^2(l_\theta + \frac{1}{2}) / [2 \sin \theta | d^2\eta_l/dl^2 |_{\theta=\theta}].\end{aligned}\quad (10)$$

In this formula we have set the impact parameter, b (distance of prolonged line of initial approach from scattering center), equal to $(l + \frac{1}{2})\lambda$, and have also distinguished explicitly between the angle of *observation*, θ (positive by convention), and the classical deflection *function*, $\Theta(l)$, (positive for net repulsion, negative for net attraction). The positive quantity l_θ is defined by the relation $\Theta(l_\theta) = \pm\theta$.

In the integral of Eq. (7), constructive interference occurs only near the l -value of stationary phase, $l = l_\theta$, where the first derivative of one or the other exponent vanishes,

$$(d\eta_l/dl)_{l_\theta} = \frac{1}{2}\Theta(l_\theta) = \frac{1}{2}\theta \quad \text{or} \quad -\frac{1}{2}\theta \quad (11)$$

(Table I). Destructive interference begins for those l -values where the curve, η_l , differs from the line which is tangent at l_θ by an amount significantly more than one radian (Fig. 1). In the region of constructive interference the curve, η_l , is replaced by its osculating parabola. Expression (7) becomes a Gauss-Fresnel integral. In this approximation the scattering amplitude in either case—attraction or repulsion—is found to have the value

$$f_{sc}(\theta) = \lambda[(l + \frac{1}{2})/2 \sin \theta (d^2\eta/dl^2)]_{l_\theta}^{1/2} \exp(2i\alpha_\theta). \quad (12)$$

TABLE I
CASES WHERE ONE OR THE OTHER EXPONENT IN EQ. (7) HAS A STATIONARY VALUE

Classical deflection	$\Theta(l_\theta)$ is	positive	negative
Relations generally valid only for monotonic $\Theta(l)$	potential is $\Theta(l)$ for $l \rightarrow 0$ is $\Theta(l)$ for $l \rightarrow \infty$ is $d^2\eta/dl^2$ is	repulsive π $0+$ positive	attractive $-\pi$ $0-$ negative
Additional relations valid for any $\Theta(l)$, assuming “big semi-classical η ”	θ (observation angle) is $2d\eta/dl$ is contributing term in (7) Approx. value of (7)	$\Theta(l_\theta)$ $\Theta(l)$ first (12)	$-\Theta(l_\theta)$ $\Theta(l)$ second (12)

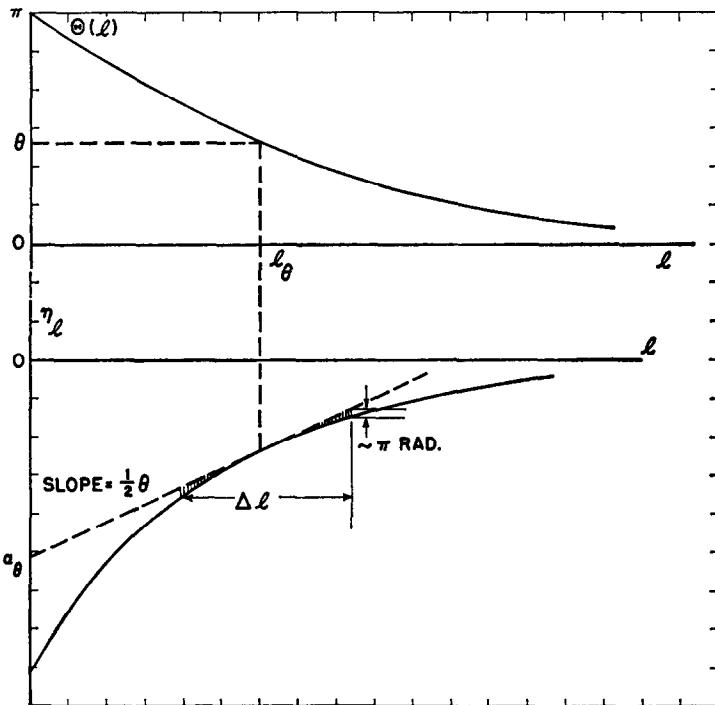


FIG. 1. Classical deflection function and phase shift for simple case of one-to-one relation between deflection and impact parameter. $\Theta(l)$ = deflection function; η_l = phase shift; l = angular momentum; θ = angle of observation; l_θ = angular momentum for classical deflection to angle of observation, i.e., $\Theta(l_\theta) = \theta$. A range of l values centered about l_θ contributes to the quantum cross section at θ , those l values being important for which the curve η_l and the line tangent to the curve at l_θ differ by less than a few radians. The semiclassical result, that the quantum and classical cross sections are equal, requires that l_θ and Δl be large compared to unity, and that the curve η_l is well represented by a parabola over the interval Δl . The phase of the quantum scattering amplitude is simply related to the intercept, α_θ , of the tangent line (Eq. 13). In the case illustrated in the diagram, α is negative.

Here the phase angle α_θ in (12),

$$\alpha_\theta = [\eta_l - (l + \frac{1}{2})(d\eta_l/dl)]_{l=l_\theta},$$

is the intercept of the tangent to the $(\eta_l, l + \frac{1}{2})$ curve with the vertical axis (Fig. 1). Since η'' may have either sign, it is more convenient to define f as the product of its absolute value and a phase factor,

$$f_{sc} = \lambda[(l + \frac{1}{2})/2 \sin \theta |\eta''|]^{1/2} e^{i\beta}, \quad (12')$$

where

$$\beta = [2\eta - 2(l + \frac{1}{2})\eta' - (2 - \eta''/|\eta''| - \eta'/|\eta'|)(\pi/4)]_{l=l_\theta}. \quad (13)$$

Although the squared absolute value of f_{sc} , Eq. (12), is equal to the classical cross section, it should be noted that the phase angle, β , is in principle accessible to measurement also, through interference with a wave scattered by the same center out of another part of the incident wave front.

This result, that $\sigma_{sc} = \sigma_{cl}$, depends upon two conditions not inherent in the semiclassical approximation itself: (a) The angle of scattering must not be too close to 0 or π ($\sin \theta$ several times greater than l_θ^{-1}). (b) There must be one and only one point of stationary phase. The latter condition will be met for all θ only if the classical deflection function, $\Theta(l)$, varies monotonically between 0 and $\pm\pi$. Such a variation is special and cannot be expected to occur often in practice. In particular the Coulomb potential is almost the only simple attractive potential with this property. This fact affords some insight into the unusual result for Coulomb potentials, $\sigma_{qu} = \sigma_{cl}$. In the next section we discuss various special features of the semiclassical cross section which can arise when the conditions of the Mott and Massey derivation are not met.

III. SPECIAL FEATURES OF SCATTERING IN SEMICLASSICAL APPROXIMATION

The important connection between classical and quantum scattering results is best seen through the classical deflection function, $\Theta(l)$, and its relation to the quantum phase shift, η_l . We are interested in this section in deflection functions for which there is not a one-to-one relation between l and Θ , or for which $\Theta(l)$ passes through 0 or π .

A. INTERFERENCE

Classically, zero, one, two, or more incident angular momenta may lead at a given energy to the same scattering angle. The total cross section is in general the sum of contributions from the different branches

$$\sigma_{cl} = \sum_i (\sigma_{cl})_i = (\sin \theta)^{-1} \sum_i b_i / |d\Theta/d\theta|_i, \quad (14)$$

where $b_i = (l_i + \frac{1}{2})\hbar/mv$ is one of the impact parameters that satisfy the condition $(2d\eta/dl)_{l_i} = \theta$. When these branches are sufficiently well separated, each will give a separate contribution to the quantum scattering amplitude which may be evaluated by the method of stationary phase.

The total semiclassical scattering amplitude will then be

$$f_{sc} = \sum_j (\sigma_{cl})_j^{1/2} \exp(i\beta_j), \quad (15)$$

where β_j is the phase angle β , defined by (13), evaluated for the j th contributing branch. For example, for two branches only,

$$\tau_{sc} = |(\sigma_{cl})_1^{1/2} + (\sigma_{cl})_2^{1/2} \exp[i(\beta_2 - \beta_1)]|^2. \quad (16)$$

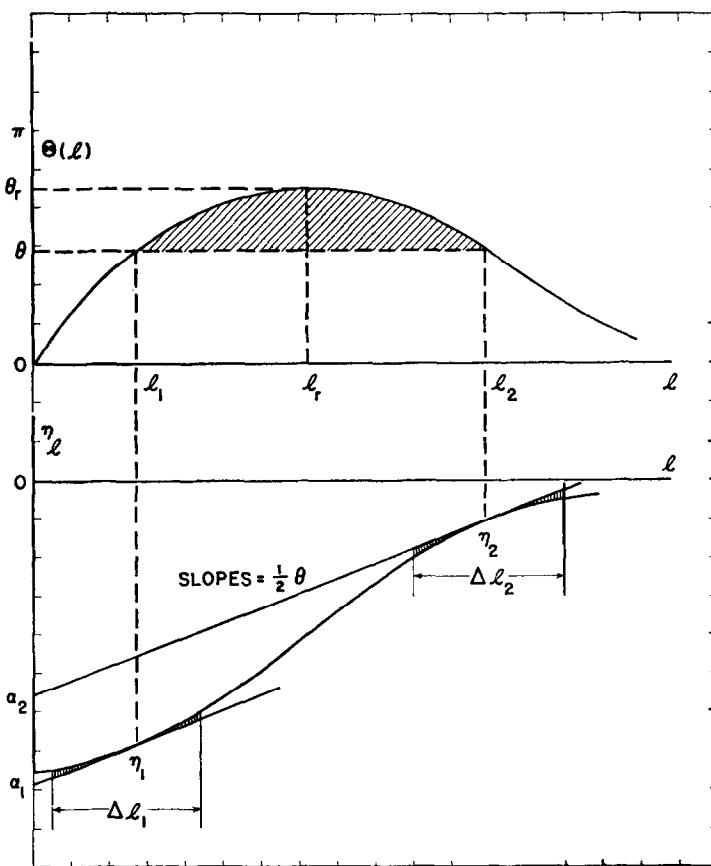


FIG. 2. Classical deflection function and phase shift illustrating interference between two branches of deflection function. The method of stationary phase is applied separately at l_1 and at l_2 . The semiclassical treatment requires for its validity that the contributing regions, Δl_1 about l_1 , and Δl_2 about l_2 , are each large compared to unity, and that parabolic approximations to η_l at l_1 and l_2 are valid over the intervals Δl_1 and Δl_2 . The contributing regions will then not overlap. The difference of intercepts of tangents, $\alpha_2 - \alpha_1$, is simply related to the phase difference of the interfering amplitudes (see Eq. 16). The shaded area under the classical deflection function is equal to $2(\alpha_2 - \alpha_1)$. (The illustrated deflection function also shows a rainbow angle, θ_r , at angular momentum l_r .)

This situation is illustrated schematically in Fig. 2. The phase difference, $\beta_2 - \beta_1$, has a simple pictorial interpretation in a graph either of $\Theta(l)$ or of η_l . In the former ($\beta_2 - \beta_1 + \pi/2$) is the area between the curve, $\Theta(l)$, and the line $\Theta = \theta$. In the latter, it is twice the difference of intercepts of the tangents to the η_l curve at the points of stationary phase.

For two contributing branches, therefore, the cross section will oscillate between the limits or envelopes,

$$\sigma_{\max} = [(\sigma_{\text{el}})_1^{1/2} + (\sigma_{\text{el}})_2^{1/2}]^2$$

and

$$\sigma_{\min} = |(\sigma_{\text{el}})_1^{1/2} - (\sigma_{\text{el}})_2^{1/2}|^2.$$

The "wavelength" of the oscillation, i.e., the angular increment in θ required to go from σ_{\max} to σ_{\min} and back to σ_{\max} , will be,

$$\delta\theta = 2\pi / |l_2 - l_1|, \quad (17)$$

where l_2 and l_1 are the points of stationary phase (Fig. 2).

It is interesting that the observed cross section can in principle be decomposed into the separate contributing branches and the classical deflection function constructed for each, provided a semiclassical description is possible. In the two-branch case, the observed σ_{\max} , σ_{\min} , and the angular separation of successive maxima give three quantities as functions of the angle of observation, θ :

$$l_1/(d\Theta/dl)_1, \quad l_2/(d\Theta/dl)_2,$$

and $(l_2 - l_1)$. These provide sufficient information to construct both branches of the deflection function, $\Theta(l)$. For more than two branches, it would also be possible in principle to construct the deflection function from the observed scattering, but in practice more or less difficult. (Figure 15 of the following paper (6) illustrates a calculated case of scattering of K^+ ions by A atoms where it is not difficult to decompose a scattering curve into *three* branches.) Finally, from a knowledge of the deflection function for all the branches, the potential may in principle be constructed (7').

B. RAINBOW SCATTERING

When the classical deflection function is nonmonotonic, contributing two or more branches to the same deflection angle, it follows that $\Theta(l)$ must possess either singularities or maxima or minima. Singularities in $\Theta(l)$ are possible and will be discussed in Part D, but smooth maxima or minima at which $d\Theta/dl = 0$ are expected to be more common. The simplest potential giving rise to such behavior is a monotonic attractive potential finite at the origin. The deflection for $l = 0$ and for $l = \infty$ is zero, and is negative in between, with one or more minima.

Since the classical cross section contains a factor $(d\Theta/dl)^{-1}$, it will have a singularity when $(d\Theta/dl)$ vanishes. This phenomenon in optics being responsible for rainbows, the name *rainbow angle* is appropriate for such an external of the deflection function. We refer to the scattering in the neighborhood of a rainbow angle as *rainbow scattering*.

Near a rainbow angle, the deflection function may be expanded in the form

$$\Theta(l) = \theta_r + q(l - l_r)^2, \quad (18)$$

where θ_r , l_r , and q have obvious meanings. On the bright side of the rainbow angle, the classical intensity will be

$$\sigma_{cl} = (\lambda^2(l_r + \frac{1}{2})/\sin \theta_r) |q(\theta - \theta_r)|^{-1/2}, \quad (19)$$

and on the dark side, the classical intensity will be zero (assuming no additional contributing branches). Exactly the same results follow from geometrical optics for the scattering of light from water droplets near a rainbow angle.

Far from the rainbow angle, on its bright side, the semiclassical cross section may be found as in Part A, considering the interference between the two branches. Near the rainbow angle, however, the amplitude contributions from the two branches overlap and cannot be computed independently. Moreover, it is no longer sufficient to fit the phase shift curve, η_l , by means of a parabola, since $d^2\eta_l/dl^2$ is approaching zero and the third derivative term must therefore be included.

The analysis of the corresponding problem in optics was carried out long ago in the famous work of Airy (1). He found on the dark side of the rainbow angle not complete blackness, but a fall-off of intensity more rapid than exponential, and on the bright side an oscillatory behavior that corresponds under low resolution to the geometrical-optical prediction. The oscillation, of course, originates in the interference between the two branches of the classical deflection curve. In the rainbow scattering of material particles, the results do not differ in any essential way from the results of Airy's analysis.

If we take the approximation (18) for the deflection function near the rainbow angle θ_r , then the phase shift η_l will be given near l_r by the expression

$$\eta_l = \eta_r \pm \frac{1}{2}\theta_r(l - l_r) + \frac{1}{6}q(l - l_r)^3. \quad (20)$$

For $\theta_r > 0$, the dominant contribution to the expression (7) for the scattering amplitude will come from the second term containing the factor $\exp(i\varphi_-)$. Substitution of (20) into (7) then leads to the formula

$$f_{sc}(\theta) \cong \left(l_r + \frac{1}{2} \right)^{1/2} \lambda (2\pi \sin \theta)^{-1/2} e^{i\delta} \int_{-\infty}^{\infty} \exp[i(\theta_r - \theta)(l - l_r) + i(q/3)(l - l_r)^3] d(l - l_r), \quad (21)$$

where the phase, δ , is given by the expression

$$\delta = 2\alpha_r - \pi/4 + (l_r + \frac{1}{2})(\theta_r - \theta), \quad (22)$$

and α_r is defined under (12). The integral in (21) is the same as that studied by

Airy, and is today designated as the Airy integral, Ai . In this notation the scattering amplitude near a rainbow angle has the form

$$f_{sc} = \lambda [2\pi(l_r + \frac{1}{2})/\sin \theta]^{1/2} q^{-1/3} e^{i\delta} \text{Ai}(x), \quad (23)$$

where x is a measure of the deviation from the rainbow angle. For positive $\Theta(l_r)$, δ is given by (22) and x is defined by the formula

$$x = q^{-1/3}(\theta_r - \theta), \quad (24)$$

regardless of whether θ is greater or less than θ_r . For $\Theta(l_r) < 0$, $\theta_r - \theta$ is replaced by $\theta - \theta_r$ in both (22) and (24). Note that the total phase of the rainbow amplitude (23) may be either δ or $\delta + \pi$, according as the product $q^{-1/3} \text{Ai}(x)$ is positive or negative (either factor may have either sign).

Provided there is no significant interference of the rainbow amplitude with amplitudes from other branches of the deflection function, the differential cross section near the rainbow angle has the form

$$\sigma_{sc} = \lambda^2(l_r + \frac{1}{2})(2\pi/\sin \theta) |q^{-2/3}| \text{Ai}^2(x). \quad (25)$$

The Airy integral, $\text{Ai}(x)$, is defined (8) by

$$\text{Ai}(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \exp \left[ixu + \frac{1}{3} iu^3 \right] du. \quad (26)$$

Other useful representations and properties are

$$\text{Ai}(x) \approx \pi^{-1/2}(-x)^{-1/4} \cos[(2/3)(-x)^{3/2} - (\pi/4)] \quad \text{for } x \rightarrow -\infty; \quad (27)$$

$$\text{Ai}(x) \cong 3^{5/6}(2\pi)^{-1}\Gamma(4/3) - 3^{1/6}(2\pi)^{-1}\Gamma(2/3)x + \dots \quad \text{for small } |x|; \quad (28)$$

$$\text{Ai}(x) \approx 2^{-1}\pi^{-1/2}x^{-1/4} \exp[-(2/3)x^{3/2}] \quad \text{for } x \rightarrow \infty; \quad (29)$$

$$\text{Ai}(x) = 3^{-4/3}(-x)^{1/2}\{J_{1/3}[(2/3)(-x)^{3/2}] + J_{-1/3}[(2/3)(-x)^{3/2}]\} \quad (30)$$

for negative x ;

$$= \pi^{-1}3^{-5/6}x^{1/2}K_{1/3}[(2/3)x^{3/2}] \quad \text{for positive } x; \quad (31)$$

$$d^2\text{Ai}(x)/dx^2 = x\text{Ai}(x). \quad (32)$$

A few values of the Airy function are listed in Table II. The oscillatory behavior of $\text{Ai}(x)$ on the bright side of the rainbow ($x < 0$) and the rapid fall-off on the dark side ($x > 0$) are evident in the table and in expressions (27) and (29); also the fact that (25), averaged over several close-lying resonances, reduces to the classical expression (19) as demanded by the correspondence principle.

If other branches of the deflection curve also contribute at the rainbow angle, then the rainbow amplitude, (23), must be combined with the other contributing amplitudes before the absolute square is taken. This situation occurs in the mag-

TABLE II
ABBREVIATED TABLE OF THE AIRY FUNCTION $\text{Ai}(x)$ BASED ON MILLER (8)

x	$\text{Ai}(x)$	$\text{Ai}(-x)$	x	$\text{Ai}(x)$	$\text{Ai}(-x)$
0.0	0.3550	0.3550	1.0	0.1353	0.5356
0.1	0.3292	0.3808	1.1	0.1200	0.5338
0.2	0.3037	0.4063	1.2	0.1061	0.5262
0.3	0.2788	0.4309	1.3	0.0935	0.5123
0.4	0.2547	0.4542	1.4	0.0820	0.4917
0.5	0.2317	0.4757	1.5	0.0717	0.4643
0.6	0.2098	0.4948	1.6	0.0625	0.4299
0.7	0.1892	0.5110	1.8	0.0470	0.3408
0.8	0.1698	0.5236	2.0	0.0349	0.2274
0.9	0.1519	0.5320	2.2	—	0.0961

Special values: Principal maximum, 0.5357 at $x = -1.0188$; first zero at $x = -2.3381$
first minimum, -0.4190 at $x = -3.2482$.

netic pole and ion-atom scattering examples treated in the succeeding paper (6). In the absence of other contributing amplitudes, an experimental rainbow cross section can be identified by its characteristic shape, and from it the parameters l_r , θ_r , and q can be deduced, so that the two branches of the classical deflection function for l near l_r can be constructed. When three branches contribute at the rainbow angle, the resolution still proceeds straightforwardly in the $K^+ - A$ example (6).

C. THE GLORY EFFECT

So long as the classical deflection function remains between 0 and π or between 0 and $-\pi$, the semiclassical cross section can be entirely described in terms of the classical cross section together with interference effects and rainbow scattering. If the deflection function passes smoothly through 0, or through $\pm\pi$, etc., a new effect arises. Classically, the vanishing of $\sin \Theta(l)$ (vanishing of element of solid angle) where l is finite and $d\Theta/dl$ is finite leads to a singularity in the cross section for forward or backward scattering. In this case we shall again take over the language of optics and meteorology and speak of a *glory*.³

We consider for definiteness a backward glory. Then the deflection function near π may be approximated by the expression

$$\Theta(l) = \pi + a(l - l_g). \quad (33)$$

³ A glory may sometimes be seen in powerful backscattering of solar radiation from the mist beneath one's plane, just around its shadow.

The classical cross section in the backward direction is then the sum of two equal contributions from $\Theta > \pi$ and $\Theta < \pi$, and is given by

$$\sigma_{\text{cl}} = 2\lambda^2 l_g |a|^{-1} (\pi - \theta)^{-1}. \quad (34)$$

When the angle of observation is sufficiently far removed from π , the semiclassical cross section for scattering in the presence of a glory may be found simply by the interference method described in Part A: the two contributing amplitudes at $\Theta(l) = \theta$ and $\Theta(l) = 2\pi - \theta$ are evaluated separately by the method of stationary phase and combined with appropriate phases. For the angle of observation near π , this method fails on two counts. First, the contributing parts of the scattering amplitude integral are not separated, but overlap. Second, the sinusoidal approximation (5) for the Legendre function must be replaced by the Bessel function approximation (6).

We may integrate (33) to obtain a suitable approximate expression for the phase shift for those values of l that contribute most to a glory:

$$\eta_l = \frac{1}{2}\pi(l - l_g) + \frac{1}{4}a(l - l_g)^2 + \eta_g. \quad (35)$$

The scattering amplitude becomes

$$f_{\text{sc}} = (\lambda/2i) \exp(2i\eta_g - \pi il_g) \int_0^\infty (2l+1) \exp[(1/2)ia(l-l_g)^2] J_0(l \sin \theta) dl. \quad (36)$$

The integral in (36) may be evaluated by using an integral representation for $J_0(x)$,

$$J_0(x) = \frac{1}{2\pi} \int_0^{2\pi} e^{ix\cos \varphi} d\varphi,$$

inverting the order of integration, and extending the lower limit of the l -integral to $-\infty$, as is permissible when al_g^2 is much greater than unity. The result is

$$f_{\text{sc}}(\theta) = \lambda(l_g + \frac{1}{2})(2\pi/a)^{1/2} e^{i\xi} J_0(l_g \sin \theta), \quad (37)$$

where the phase constant ξ is given by the formula

$$\xi = 2\eta_g - \pi l_g - \pi/4 \quad (38)$$

for a backward glory. For a forward glory the result is the same except that the term πl_g in (38) is missing. Notice that ξ is the total phase of f only if a and J_0 are positive. Otherwise terms $\pi/2$ or π or both must be subtracted from ξ to give the total phase if a or J_0 or both are negative. In case there are no other amplitudes interfering with (37), the glory cross section is given by the formula

$$\sigma_{\text{sc}} = \lambda^2 (l_g + \frac{1}{2})^2 (2\pi/|a|) J_0^2(l_g \sin \theta). \quad (39)$$

The singularity in the classical cross section is replaced by a finite peak in the forward or backward direction of magnitude

$$\sigma_{sc}(\text{peak}) = \lambda^2(l_0 + \frac{1}{2})^2(2\pi/|a|).$$

The oscillations predicted by the Bessel function may be said to arise from interference of the contributions from the two branches of the deflection function near a glory,

$$\Theta > \pi \text{ (or } 0) \text{ and } \Theta < \pi \text{ (or } 0).$$

When the intensity is averaged over several such oscillations by way of the formula $\langle J_0^2(x) \rangle = (1/\pi x)$, then Eq. (39) reduces to the classical formula (34) for scattering due to a glory.

D. ORBITING, OR SPIRAL SCATTERING

Rainbow angles and glories arise when the classical deflection function, $\Theta(l)$, possesses relative maxima or minima, or passes with finite slope through $0, \pm\pi, \dots$. In addition, the deflection function may have a singularity at some critical value, l_1 , corresponding to an infinite spiralling of the classical orbit toward a limiting circular orbit. This phenomenon is familiar in atomic collisions—for example, in the low energy collision between a rare gas atom and an ion in a rare gas configuration—and has been given the name *orbiting* (9).⁴ The corresponding phenomenon in optics is not familiar and appears not to have been named.

Orbiting arises when the effective potential for the radial motion possesses, for some angular momentum l_1 , a relative maximum equal to the available energy:

$$\left(\frac{dV_{\text{eff}}(l_1)}{dr} \right)_{r_1} = 0, \quad V_{\text{eff}}(r_1, l_1) = E. \quad (40)$$

Under these circumstances, the classical deflection function will vary logarithmically near l_1 (Fig. 3) :

$$\begin{aligned} \Theta(l) &= \theta_1 + b \ln \left(\frac{l - l_1}{l_1} \right), & l > l_1, \\ \Theta(l) &= \theta_2 + 2b \ln \left(\frac{l_1 - l}{l_1} \right), & l < l_1. \end{aligned} \quad (41)$$

⁴ A discussion of classical orbiting and a summary of literature on classical deflection theory and deflection calculations appear in Section 8.4 prepared jointly with E. L. Spotz. Section 10.3 by J. deBoer and R. B. Bird summarizes the mathematical expression of total cross sections as *power series* in Planck's constant, a type of analysis not suitable for the rapidly oscillating *differential cross section*.

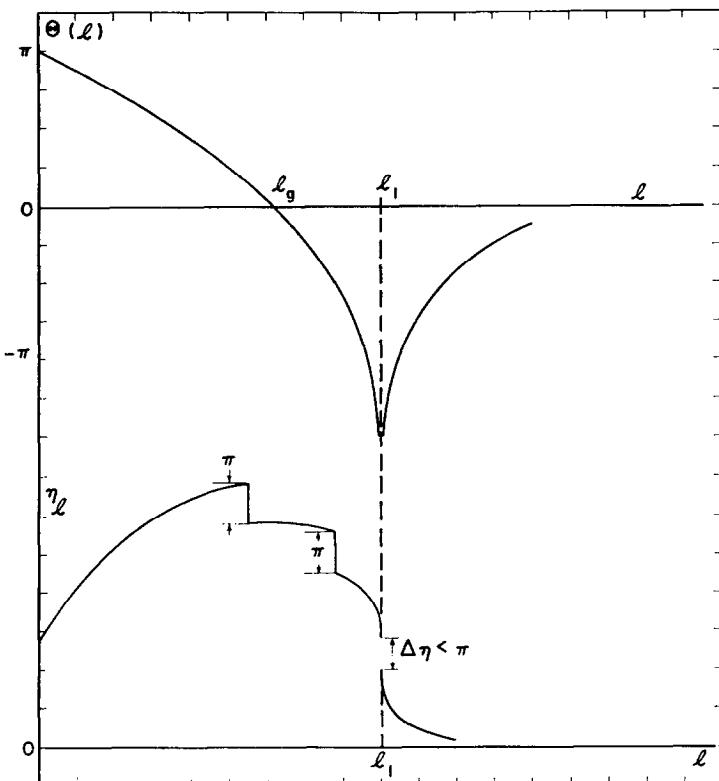


FIG. 3. Classical deflection function and phase shift illustrating the phenomenon of orbiting. Near the critical angular momentum, l_1 , the deflection function and the phase shift have a characteristic dependence on $l - l_1$ (Eqs. 41 and 44). At l_1 the phase shift has infinite slope, and suffers a discontinuity less than π . For $l < l_1$, the phase shift may have a number of discontinuities, each of magnitude π , corresponding to resonance levels within the barrier. The phenomenon of barrier penetration makes the jumps in η_l not absolutely sharp. (The deflection function illustrated in this figure also gives a rise to a forward glory, owing to the smooth passage of $\Theta(l)$ through zero at $l = l_g$).

For l somewhat greater than l_1 , the particle will spiral in and out, not quite reaching the barrier top. For l somewhat less than l_1 , the centrifugal barrier will be lower and the particle will spiral over the barrier, into an inner region, and out over the barrier again. The constants θ_1 and θ_2 in (41) may differ by an arbitrary amount, according to the nature of the potential *within* the barrier. The barrier itself may arise from a real barrier in the potential, $V(r)$, or merely from the centrifugal barrier itself if the potential is attractive and weakens rapidly with increasing r .

The classical cross section arising from orbiting will be the sum of two parts,

from $l > l_1$ and $l < l_1$. Each part will be a superposition of an infinite number of terms arising from successive intervals $\Theta = 0$ to $-\pi$, $-\pi$ to -2π , etc. Each term in the series will be much smaller than the preceding term. The major contribution, for $0 > \Theta = -\theta > -\pi$, will be

$$\sigma_{el}^{(1)} = \lambda^2 (l_1 + \frac{1}{2})^2 (b \sin \theta)^{-1} (e^{-(\theta+\theta_1)/b} + \frac{1}{2} e^{-(\theta+\theta_2)/2b}), \quad (42)$$

showing an exponential decrease with increasing angle. Successive terms may be obtained from (42) by replacing θ by $2\pi - \theta$, $2\pi + \theta$, $4\pi - \theta$, $4\pi + \theta$, \dots . Quantum mechanically there will be interference among all of these terms, and between the two terms in (42). For small b , however, a single term may be dominant.

The constant b , measuring the rate of fall-off of the cross section, may be related to the physical parameters of the problem:

$$b = [2V_l/r^2 | V''_{eff} |]^{1/2}. \quad (43)$$

V''_{eff} is the curvature of the effective potential (centrifugal plus actual) and V_l is the centrifugal potential alone, both evaluated at r_1 , l_1 .

If barrier penetration is ignored, the conditions for a semiclassical analysis can never be met throughout the whole region of orbiting. The phase shift in the primitive JWKB approximation varies neither slowly nor smoothly near $l = l_1$. It approaches an infinite slope near l_1 and suffers a finite discontinuity at l_1 . On the high- l side of l_1 , for example, the phase shift is approximately,

$$\eta_l = \eta_1 + \frac{1}{2}\theta_1(l - l_1) + \frac{1}{2}b(l - l_1)[\ln(l - l_1)/l_1] - 1, \quad (44)$$

a result equivalent to the primitive JWKB phase shift given by Eq. (27) of the preceding paper (10). In that paper, the dependence of η on energy for fixed l was considered. In the present analysis, with fixed energy and variable l , let ϵ represent the energy difference between the fixed energy and the variable height of the barrier, in units of $\hbar\omega_{inverted}$, the characteristic energy of the inverted oscillator potential. Then, approximately, for small ϵ ,

$$\epsilon = -b(l - l_1),$$

with b defined by (43). This establishes the connection between Eq. (44) above and Eq. (27) in Ref. 10. (Note that η_1 does not have the same meaning in the two equations.)

We conclude that there is no semiclassical approximation to the orbiting effect of simplicity or generality comparable to the analysis for rainbow scattering and glory scattering. In any particular problem involving orbiting, it is necessary to correct the JWKB phase shift for transition effects associated with the barrier maximum, and for resonance effects associated with virtual bound states. These effects are analyzed in Eq. (21) and especially in Fig. 4 of the preceding paper

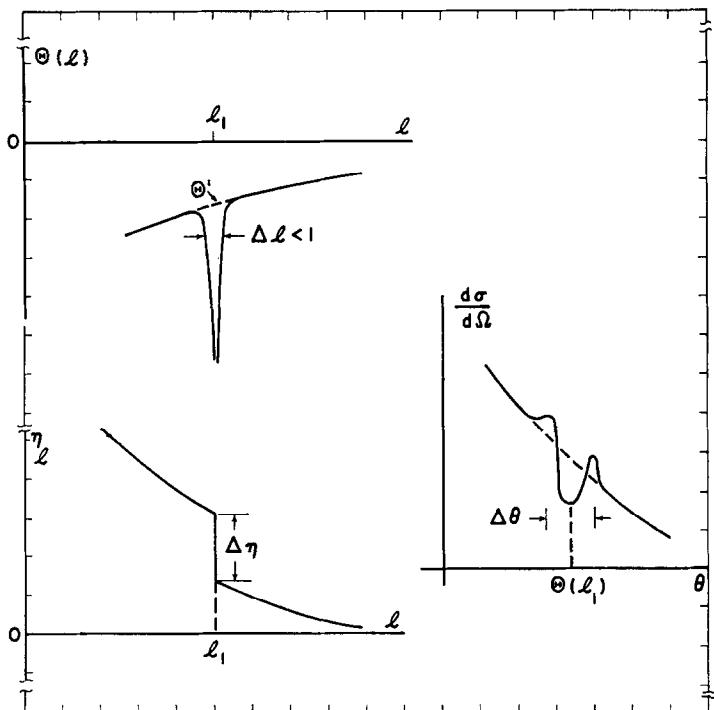


FIG. 4. Approximation of sharp orbiting spike. If the singular behavior of $\Theta(l)$ near l_1 is condensed into an interval $\Delta l < 1$, the classical orbiting phenomenon influences the quantum cross section only through a discontinuity, $\Delta\eta$, in η_l at l_1 . The differential cross section then shows a minimum (Eq. 45) at $\theta = \Theta'(l_1)$, and a "disturbance" over an angular interval $\delta\theta \sim [d\Theta'/dl]_{l_1}^{1/2}$. Here Θ' stands for the smoothed deflection function that ignores the orbiting spike (the dashed curve in the graph of $\Theta(l)$ versus l).

(10), as a function of energy, for a given l . From the results one can construct a curve for phase shift as a function of l for a given energy [approximately by the substitution $\epsilon = -b(l - l_1)$], a curve that will have a character very different according as the barrier is thin (large value of the parameter n_1 of Ref. 10) or thick (small n_1). Having this curve for the particular problem, one can examine the scattering integral (7) and decide what approximate method, if any, is suitable for its evaluation. We content ourselves here with mentioning several possible limiting situations.

(a) Sharp Spike

It is possible that the whole orbiting phenomenon occurs in an angular momentum interval $\Delta l < 1$. Then the exponential type cross section (42) is completely washed out in the quantum cross section, but the spike still makes itself

felt by introducing a discontinuity in the phase shift (see Fig. 4). The range of l values contributing to the scattering is $\delta l \sim [d^2\eta_l/dl^2]^{-1/2}$. Hence if $|l_0 - l_1| \gtrsim \delta l$, where $|\Theta(l_0)| = \theta$, the orbiting spike will have no influence. If $|l_0 - l_1| \lesssim \delta l$, the spike will influence the scattering. In particular, for $l_0 = l_1$, the cross section will be diminished:

$$\sigma_{sc} = \frac{1 + \cos 2\Delta\eta}{2} \sigma_{el}, \quad (45)$$

where σ_{el} refers to the cross section at l_1 in the absence of a spike. The total angular width of the "disturbed" region of the cross section is $\delta\theta \sim [d\Theta(l)/dl]_{l_1}^{1/2}$ (evaluated in the absence of the spike). Figure 4B of Ref. 10 might represent sharp spike behavior.

(b) Thin Barrier

An opposite sort of approximation is possible when barrier penetration is very important (see Fig. 5). If the barrier is "thin" and the inner well is "thick", the resonance levels will overlap and merge into a continuum. The infinite slope of the primitive JWKB phase shift is smoothed into a finite slope. For a sufficiently thin barrier the phase shift will have small enough slope to be treated everywhere semiclassically. It will have the form,

$$\eta_l = \eta_1 + \left(\frac{d\eta}{dl}\right)_1 (l - l_1) + \frac{q}{6} (l - l_1)^3, \quad (46)$$

i.e., exactly the rainbow form. Although barrier penetration has no classical analog, we may define a "classical deflection function" $\Theta(l) = 2(d\eta_l/dl)$, and interpret $(d\eta/dl)_1$ as one-half the rainbow angle. In this limit, the classical orbiting will appear quantum-mechanically as a rainbow effect. Figure 4D of Ref. 10 could represent thin barrier behavior.

The barrier penetration will always have the effect of converting the infinite spike in the classical deflection function into a finite peak. Whether this implies a rainbow behavior depends on the width of the peak in l -units, and the degree of smoothing introduced by the barrier penetration.

(c) Thick Barrier

If the barrier penetration is unimportant and the top of the barrier is so broad that very many l -values are involved in the rapidly rising part of the deflection function, then the contributions of the two branches of the deflection function may be treated separately semiclassically, by the method of stationary phase, and the resulting amplitudes added before squaring—i.e., it is a simple interference problem. One may note from (42), however, that the two amplitudes are expected to be generally quite different in magnitude. Therefore, the interference

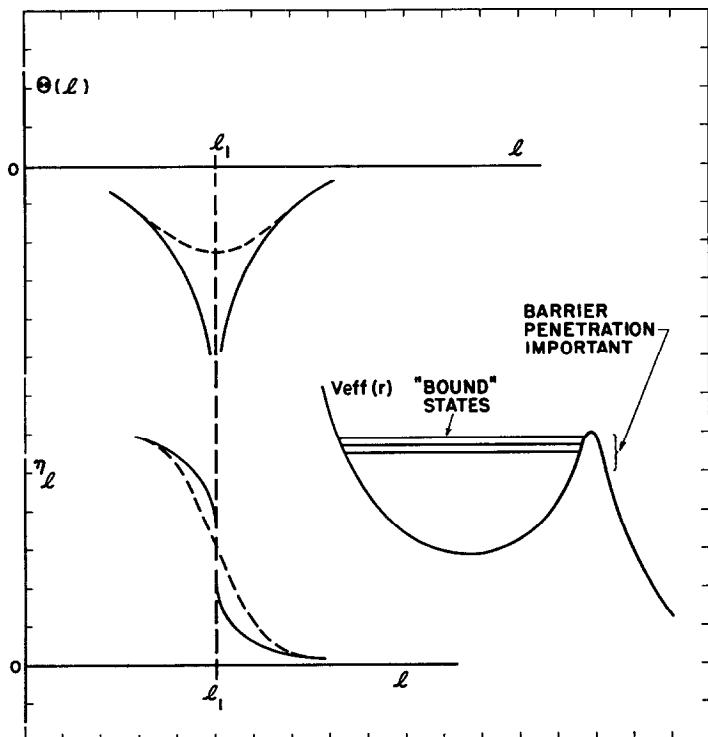


FIG. 5. Approximation of thin barrier. Sufficiently great penetrability of the barrier in V_{eff} , coupled with overlapping resonances within the barrier, causes the phase shift to be smoothed, and the maximum slope of the phase shift to be reduced to a value small enough to permit a rainbow approximation. A modified "classical deflection function," defined by $\Theta = 2d\eta_l/dl$, shows a smooth minimum instead of the singularity associated with classical orbiting.

pattern should be weak, and the observed cross section should follow approximately the exponential angular dependence of the larger classical branch.

E. TRANSITION FROM ORBITING TO RAINBOW ANGLE SCATTERING; BEHAVIOR NEAR A CRITICAL POINT

Special attention is given in the examples of the following paper to the scattering of an ion by an atom, or an atom by an atom, at one particular energy, where rainbow angle scattering occurs. At lower energy orbiting occurs. The transition from one behavior to the other, from orbiting to rainbow angle scattering, at a critical energy E_{crit} , is a phenomenon not at all special to this particular problem, and is to be expected in any system which manifests orbiting at low enough energies. The following considerations on this transition will be limited

to the analysis of the classical deflection function Θ and the semiclassical equivalent of a phase shift, η_{sc} , near the transition, and some general remarks on the implications for the quantum theory phase shift, η . No attempt will be made to give a formula for the cross section valid in the neighborhood of the critical point. Here the condition is not fulfilled for a semiclassical formula. The scattering amplitude is not the sum of many partial waves with slowly varying phase shifts.

To attain the critical point the particles of reduced mass m must collide with a particular momentum p_1 and a particular impact parameter b_1 :

$$\begin{aligned} E_{\text{crit}} &= p_1^2/2m, \\ l_{\text{crit}} &= p_1 b_1/\hbar. \end{aligned} \quad (47)$$

These conditions are just such that the particle fails to find a potential barrier. In other words, at the separation $r = r_1$ where the approaching particles are turned back, the energy, $p_r^2/2m = E - V(r) - (l + \frac{1}{2})^2\hbar^2/2mr^2$, of the radial motion varies with r , not quadratically as at the top of a barrier, but cubically:

$$(k_r^{(1)})^2 = \hbar^{-2}(p_r^{(1)})^2 = a(r - r_1)^3 + \text{higher order terms.} \quad (48)$$

Introduce the abbreviation $v(r) = 2m\hbar^{-2}V(r)$ for the "reduced potential." Then the radial wave number for the critical collision is given by the formula

$$(k_r^{(1)})^2 = k_1^2 - v(r) - (l_1 + \frac{1}{2})^2/r^2. \quad (49)$$

Equating (48) and (49), we obtain an expression for the potential near the critical point. With its help we find the radial momentum for a collision (k, l) which is *not* the critical collision:

$$k_r^2 = k^2 - v(r) - (l + \frac{1}{2})^2/r^2 \quad (50)$$

$$\cong (k^2 - k_1^2) - [(l + \frac{1}{2})^2 - (l_1 + \frac{1}{2})^2]/r^2 + a(r - r_1)^3 \quad (51)$$

$$\cong a(x^3 + 3\lambda x + 2\epsilon) = a(x - x_a)(x - x_b)(x - x_c), \quad (52)$$

where $x = r - r_1$, and the parameters which measure the angular momentum excess and the energy excess, relative to the triple point, are

$$\lambda = (2/3ar_1^3)[(l + \frac{1}{2})^2 - (l_1 + \frac{1}{2})^2], \quad (53)$$

$$\epsilon = (1/2a)\{(k^2 - k_1^2) - [(l + \frac{1}{2})^2 - (l_1 + \frac{1}{2})^2]/r_1^2\}. \quad (54)$$

The approximate expressions (51) and (52) are appropriate only for k near k_1 , l near l_1 , and r near r_1 .

We recall the semiclassical approximate formula for the phase shift, Eq. (3) (the primitive JWKB phase shift of Ref. 10). We divide the integration interval into a part from the turning point, r_0 , to some radius, r_2 , in which the approximate expression (52) may be used, and a part from r_2 to ∞ in which the exact

expression (50) must be used. The radius r_2 is chosen small enough so that (52) is valid, but large enough so that the cubic term in (52) is much greater than the linear and constant terms. One may then obtain an approximate expression for the semiclassical phase shift, η_{sc} , near the critical wave number, k_1 , and critical angular momentum, l_1 , accurate to leading order in the angular momentum and energy excess. This expression is most naturally written as the sum of two parts,

$$\eta = \eta_{\text{reg}} + \eta_{\text{TP}}. \quad (55)$$

The first part is regular in its analytic behavior near the triple point,

$$\begin{aligned} \eta_{\text{reg}} = \eta_1 + (l - l_1)(\pi/2) - \frac{1}{2}[(l + \frac{1}{2})^2 \\ - (l_1 + \frac{1}{2})^2]J_\lambda + (1/2k_1)(k^2 - k_1^2)J_\epsilon, \end{aligned} \quad (56)$$

and depends upon the form of the potential far from the triple point. This dependence shows in the following three constants, each of which measures a distinct feature of the critical orbit:

$$\begin{aligned} \eta_1 &= \lim_{R \rightarrow \infty} \left\{ \int_{r_1}^R k_r^{(1)} dr - \int_{(l_1+1/2)/k_1}^R \left[k_1^2 - \left(l_1 + \frac{1}{2} \right)^2 / r^2 \right]^{1/2} dr \right\}; \\ J_\lambda &= \int_{r_1}^\infty \left[\frac{1}{r^2 k_r^{(1)}} - \frac{1}{r_1^2 a^{1/2}(r - r_1)^{3/2}} \right] dr; \\ J_\epsilon &= -r_1 + \int_{r_1}^\infty \left[\frac{k_1}{k_r^{(1)}} - \frac{k_1}{a^{1/2}(r - r_1)^{3/2}} - 1 \right] dr. \end{aligned} \quad (57)$$

The second part of the phase shift, η_{TP} , is characteristic of the triple point, not of the remote portions of the potential, and depends sensitively upon the parameters of angular momentum and energy excess:

$$\begin{aligned} \eta_{\text{TP}} = a^{1/2} \lim_{x \rightarrow \infty} \left\{ \int_{\text{TP}}^x (x^3 + 3\lambda x + 2\epsilon)^{1/2} dx - (2/5)x^{5/2} - 3\lambda x^{1/2} \right. \\ \left. + 2\epsilon x^{-1/2} \right\} = a^{1/2}(2|\lambda|^{1/2})^{5/2} N_\pm(\epsilon/|\lambda|^{3/2}) \\ \begin{cases} N_+ \text{ for positive } \lambda \\ N_- \text{ for negative } \lambda \end{cases}. \end{aligned} \quad (58)$$

Here N_+ (or N_-) is a dimensionless function of the single variable $\epsilon/\lambda^{3/2}$ (or $\epsilon/(-\lambda)^{3/2}$) expressible in the form

$$N_\pm = (3^{3/4}/5)A^{-1/4}[B E(m) + C K(m)]. \quad (59)$$

Table III gives the coefficients A , B , C , in this formula and the modulus $m = k^2$

TABLE III

Parametric expressions for (1) the roots x_a, x_b, x_c of the dimensionless measure of kinetic energy ($x^3 + 3\lambda x + 2\epsilon$) and (2) the dimensionless factor N_{\pm} in the triple point part of the phase shift (Eq. 59). The dimensionless measure of potential, $-(x^3/2) - (3\lambda/2)x$, always has an inflection at $x = 0$, but has no maximum or minimum when λ is positive. Then there exists only one real root or turning point (Case I in the table). When λ is negative, the dimensionless potential has a local minimum value $-|\lambda|^{3/2}$ at $x = -|\lambda|^{1/2}$ and a local maximum $|\lambda|^{3/2}$ at $x = |\lambda|^{1/2}$. Consequently there is again only one root when ϵ is greater than $|\lambda|^{3/2}$ (Case II in the table) or less than $-|\lambda|^{3/2}$ (Case III). Only in these three cases is one root real and the other two complex conjugate; only then is the discriminant $\lambda^3 + \epsilon^2$ positive. When this discriminant is negative (Case IV), then λ is negative, and ϵ lies between $-|\lambda|^{3/2}$ and $|\lambda|^{3/2}$. Then there are three real roots, of which only the largest represents the turning point for the collision process.

Configuration and parameter θ	Roots $ \lambda ^{-1/2}x$	A and modulus $m = k^2$	B, C : Coefficients of elliptic functions $E(m), K(m)$ in Eq. (59)
No maxima or minima; λ positive; $N = N_+$; $-\infty < \epsilon < \infty$; $\epsilon = \lambda^{3/2}$ $\sinh 3\theta$	$-2 \sinh \theta$ and $(\sinh \theta \pm i3^{1/2} \cosh \theta)$	$A = \sinh^2 \theta + \frac{1}{4}$; $m = \frac{1}{2} + (3^{1/2}/4A^{1/2}) \times \sinh \theta$; $\sin^2 15^\circ < m < \sin^2 75^\circ$	$B = -2 \cdot 3^{1/2} (\sinh^2 \theta + \frac{1}{4})^{1/2}$; $C = 3^{1/2} A^{1/2} - \sinh \theta + (\frac{1}{2}) \sinh 3\theta$
Maximum and minimum with energy above them; λ negative; $N = N_-$; $\epsilon > \lambda ^{3/2}$; $\epsilon = (-\lambda)^{3/2}$ $\cosh 3\theta$	$-2 \cosh \theta$ and $(\cosh \theta \pm i3^{1/2} \sinh \theta)$	$A = \cosh^2 \theta - \frac{1}{4}$; $m = \frac{1}{2} + (3^{1/2}/4A^{1/2}) \times \cosh \theta$; $\sin^2 75^\circ < m < \sin^2 90^\circ$	$B = 2 \cdot 3^{1/2} (\cosh^2 \theta - \frac{1}{4})^{1/2}$; $C = -3^{1/2} A^{1/2} + \cosh \theta + (\frac{1}{2}) \cosh 3\theta$
Maximum and minimum with energy below them; λ negative; $N = N_-$; $\epsilon < - \lambda ^{3/2}$; $\epsilon = -(-\lambda)^{3/2} \cosh 3\theta$	$2 \cosh \theta$ and $(-\cosh \theta \pm i3^{1/2} \sinh \theta)$	$A = \cosh^2 \theta - \frac{1}{4}$; $m = \frac{1}{2} - (3^{1/2}/4A^{1/2}) \times \cosh \theta$; $\sin^2 0^\circ < m < \sin^2 15^\circ$	$B = 2 \cdot 3^{1/2} (\cosh^2 \theta - \frac{1}{4})^{1/2}$; $C = -3^{1/2} A^{1/2} - \cosh \theta - (\frac{1}{2}) \cosh 3\theta$
Maximum and minimum with energy between them; λ negative; $N = N_-$; $-(-\lambda)^{3/2} < \epsilon < (-\lambda)^{3/2}$; $\epsilon = -(-\lambda)^{3/2} \cos 3\theta$	a: $2 \cos(\theta + 120^\circ)$; b: $2 \cos(\theta - 120^\circ)$; c: $2 \cos \theta$, $x_a < x_b < x_c$, $0^\circ < \theta < 60^\circ$	$A = \sin^2(\theta + 60^\circ)$; $m = [\sin \theta / \sin(\theta + 60^\circ)]$; $\sin^2 0^\circ < m < \sin^2 90^\circ$	$B = 3^{1/2} \sin(\theta + 60^\circ)$; $C = -\cos \theta - (\frac{1}{2}) \cos 3\theta$

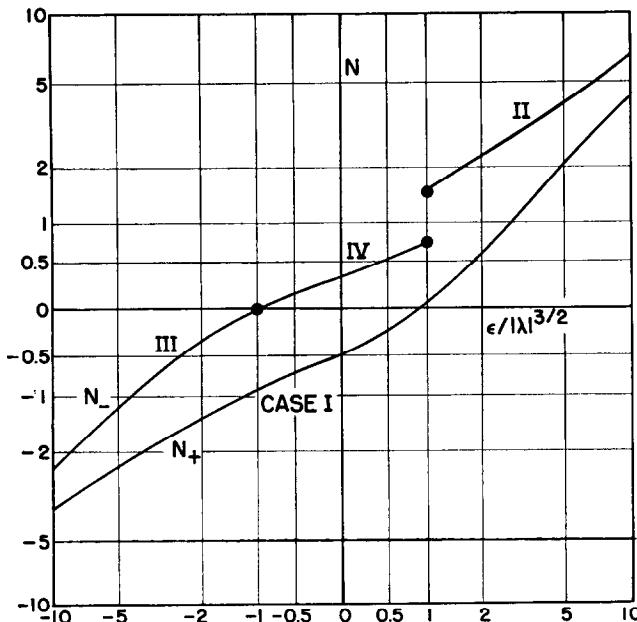


FIG. 6. Dimensionless factors N_+ and N_- for the triple point part, η_{TP} (Eqs. 58 and 59) of the phase shift (Eq. 55) as a function of the dimensionless measure of energy, $\epsilon/|\lambda|^{3/2}$. The scattering potential has one maximum and one minimum when λ is negative—hence the discontinuous change in the phase shift on crossing the barrier maximum.

of the familiar complete elliptic integrals⁵ K and E of the first and second kind, respectively.

Figure 6 shows the dimensionless factors N_{\pm} in the triple point phase shift as a function of the energy-proportional parameter $\epsilon/|\lambda|^{3/2}$. There is a jump in the curve for N when the energy rises across the value $\epsilon = |\lambda|^{3/2}$. Then the colliding particle is first able to surmount the potential maximum that occurs for negative λ and reach to the left of this barrier into the region of the potential minimum. The jump in the phase shift at this point is measured by the phase integral for vibratory motion *within* the minimum with energy parameter $\epsilon = |\lambda|^{3/2}$.

$$\begin{aligned}\Delta\eta_{TP} &= a^{1/2} \int_{\text{single root}}^{\text{double root}} (x^3 - 3|\lambda|x + 2|\lambda|^{3/2})^{1/2} dx \\ &= (4 \cdot 3^{3/2}/5)a^{1/2}|\lambda|^{5/4}; \\ \Delta N_- &= N_-(1+) - N_-(1-) = (3/5)(3/2)^{1/2} = 0.735.\end{aligned}\quad (60)$$

⁵ We use the notation of Milne-Thomson (11) who defines the modulus m equal to the square of the usual parameter k .

The analytic behavior of the JWKB phase shift near this jump point is useful in estimating true phase shifts for the orbiting process. Just above the discontinuity

$$\begin{aligned}\eta_{\text{TP}} \doteq & a^{1/2} (2|\lambda|^{1/2})^{5/2} [(3/5)6^{1/2} + (6^{1/2}/24) \\ & + (6^{1/2}/24)\Delta \ln(864e/\Delta)]\end{aligned}\quad (61)$$

and just below

$$\begin{aligned}\eta_{\text{TP}} \doteq & a^{1/2} (2|\lambda|^{1/2})^{5/2} [(3/10)6^{1/2} \\ & + (6^{1/2}/48)(-\Delta) \ln(-864e/\Delta)]\end{aligned}\quad (62)$$

where $\Delta = \epsilon/|\lambda|^{3/2} - 1$, a measure of the energy excess above the barrier.

Finally, the classical deflection near the critical point may be obtained, as indicated in Eq. (4), by differentiating Eq. (55) for η . For this purpose Eq. (56) is used for η_{reg} ; and Eqs. (58) and (59) or Eqs. (61) and (62) for η_{TP} , according as the energy parameter ϵ is not or is close to the jump point $\epsilon_{\text{jump}} = (-\lambda)^{3/2}$.

We find,

$$\begin{aligned}\Theta &= \Theta_{\text{reg}} + \Theta_{\text{TP}} ; \\ \Theta_{\text{reg}} &= \pi - 2(l_1 + \frac{1}{2})J_\lambda ; \\ \Theta_{\text{TP}} &= -2a^{-1/2}r_1^{-2}(l_1 + \frac{1}{2})[|\lambda|^{-1/4}F_\pm(\epsilon/|\lambda|^{3/2}) \\ &\quad - 2r_1^{-1}|\lambda|^{1/4}D_\pm(\epsilon/|\lambda|^{3/2})].\end{aligned}\quad (63)$$

Here the dimensionless deflection function F_\pm and D_\pm (subscripts denoting the sign of λ) have the values,

$$F_\pm(Z) = \int_{\text{TP}}^{\infty} (u^3 \pm 3u + 2Z)^{-1/2} du, \quad (64a)$$

and

$$D_\pm(Z) = \lim_{U \rightarrow \infty} \left[\int_{\text{TP}}^U (u^3 \pm 3u + 2Z)^{-1/2} u du - 2U^{1/2} \right]. \quad (64b)$$

It is simpler to find the deflection function directly from (64) than to differentiate the expressions for the phase shift which are given in Table III. The integrals in (64) lead (12) to complete elliptic functions of the same modulus m which appears in Table III.

Other features of the potential besides the semiclassical phase shift are of interest when the potential has a local minimum and a local maximum (λ negative) and when the energy lies between these extremal values ($-|\lambda|^{3/2} < \epsilon < |\lambda|^{3/2}$).

The position of the n th *semi-stable bound level* in the potential minimum is given in the JWKB approximation by the following implicit formula for ϵ ,

$$\int_{x_a}^{x_b} a^{1/2}(x^3 + 3\lambda x + 2\epsilon)^{1/2} dx = \left(n + \frac{1}{2}\right)\pi, \quad (65)$$

where the three roots of the cubic are arranged in the order $x_a < x_b < x_c$, as in the last row of Table III. When the energy parameter is expressed in terms of θ in the form listed in the table,

$$\epsilon = -(-\lambda)^{3/2} \cos 3\theta, \quad (66)$$

then the eigenvalue equation reduces to the form

$$a^{1/2}(2|\lambda|^{1/2})^{5/2}N_{\text{bound}}(\epsilon/|\lambda|^{3/2}) = (n + \frac{1}{2})\pi, \quad (67)$$

where N_{bound} is equal to N_- [Eq. (59) and Table III, Case IV]. This quantity is replotted in Fig. 7. When the energy is only a little more than the energy of the potential minimum, the parabolic approximation is good, and the eigenvalue equation reduces to

$$a^{1/2}|\lambda|^{5/4}(\pi/3^{1/2})(|\lambda|^{-3/2}\epsilon + 1) \doteq (n + \frac{1}{2})\pi, \quad (68)$$

whence

$$N_{\text{bound}} \doteq 3^{-1/2}2^{-5/2}\pi(|\lambda|^{-3/2}\epsilon + 1). \quad (69)$$

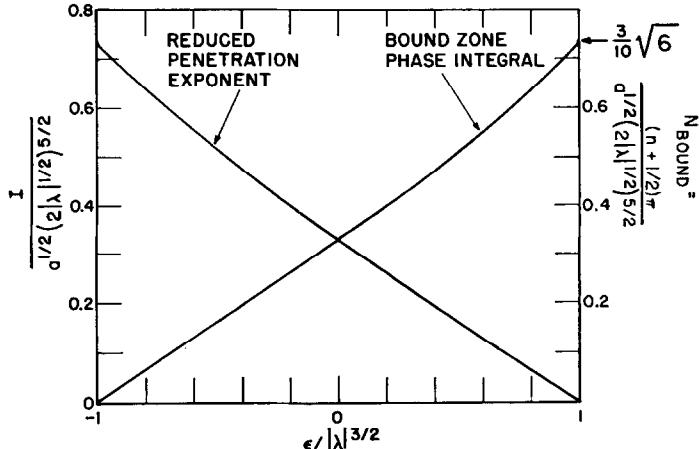


FIG. 7. Phase integral for determination of number of semistable bound states and reduced penetration factor for determination of level widths, both for case of barrier such that reduced kinetic energy is $x^3 + 3\lambda x + 2\epsilon$. (See Eqs. 67 and 77). The bound zone phase integral is identical with Section IV of the graph in Fig. 6.

Near the potential maximum the JWKB eigenvalue equation has a limiting form given by

$$(n + \frac{1}{2})\pi = \eta_{TP}[\text{Eq. (61)}]. \quad (70)$$

The typical semistable bound level has a finite mean life τ_n and a finite decay constant $A_n = 1/\tau_n$. The distribution in energy of the disintegrating systems has a spread about the characteristic energy E_n , with a full width at half maximum $\Gamma_n = \hbar A_n$. This width may be denoted by γ_n when expressed in the units of the energy parameter ϵ of Eq. (54). The JWKB approximation gives

$$\gamma_n = 1/2\pi(d\epsilon/dn)_n \exp(-2I). \quad (71)$$

The factors in this formula may be evaluated as follows. Differentiation of (65) gives

$$\pi dn/d\epsilon = a^{1/2} \int_{x_a}^{x_b} (x^3 + 3\lambda x + 2\epsilon)^{-1/2} dx, \quad (72)$$

or, in terms of the notation of the last row of Table III,

$$d\epsilon/dn = \pi 3^{1/4} 2^{-1/2} |\lambda|^{1/4} a^{-1/2} [\sin(\theta + 60^\circ)]^{1/2} / K(m). \quad (73)$$

Near the potential minimum where the motion is harmonic this general formula reduces to

$$d\epsilon/dn \doteq 3^{1/2} |\lambda|^{1/4} a^{-1/2}; \quad (74)$$

and near the summit,

$$d\epsilon/dn \doteq 2\pi 3^{1/2} |\lambda|^{1/4} a^{-1/2} / \ln[864/(1 - |\lambda|^{-3/2} \epsilon)]. \quad (75)$$

The amplitude penetration exponent I has the value

$$I = a^{1/2} \int_{x_b}^{x_c} (-x^3 - 3\lambda x - 2\epsilon)^{1/2} dx. \quad (76)$$

The potential is symmetric against the inversion $v \rightarrow -v$, $x \rightarrow -x$, at the origin. Therefore the amplitude penetration exponent is given by the equation

$$I(a, \lambda, \epsilon) = [n(a, \lambda, -\epsilon) + \frac{1}{2}]\pi = a^{1/2} (2|\lambda|^{1/2})^{5/2} N_{\text{bound}}(-\epsilon/|\lambda|^{3/2}). \quad (77)$$

Near the top of the barrier the properties of semistable bound states and their contribution to scattering can no longer be evaluated by the JWKB type of formula (67) because of characteristic quantum corrections (Ref. 10).

IV. DISCUSSION

We have found that the analysis of scattering is appreciably simplified when the conditions are satisfied for a semiclassical treatment. That description nor-

mally demands that the curve of the phase $\varphi_{\pm} = 2\eta_l \pm (l + \frac{1}{2})\theta \pm \pi/4$ as a function of l shall be well fitted at each point l_i of stationary phase by an oscillating parabola, in the following sense: The parabolic curve must agree with the actual phase shift to within a small fraction of a radian so long as the quadratic term in the parabola remains less than about a radian; and there must be an appreciable number, Δl , of l values for which this inequality is satisfied. The second part of the condition justifies the replacement of the sum by an integral and the first part ensures that this integral shall be Gaussian. There exists also a third condition, that the spread, Δl , must be small compared to l_i itself.

Of course, the Airy integral permits us to go outside the framework of the quadratic approximation and still obtain a good analytic and asymptotic formula for the scattering.

More generally, in speaking about the legitimacy of the semiclassical approximation, it is necessary to state that the manner of derivation of each formula defines in and by itself the conditions for the validity of that formula. It would be extremely complicated to make a general classification of all those curves of phase shift as function of quantum number for which these conditions are fulfilled. It is much simpler to take a given curve and ask for what angles of observation either the Gaussian or the Airy integral will reasonably well represent the scattering amplitude. Such a representation will be good only if the following three conditions are all satisfied at the same time: (1) a quadratic or a cubic formula will fit the curve $\eta = \eta_l$ over the range of l values that contribute significantly to the amplitude: $\Delta l \sim (d^2\eta/dl^2)^{-1/2}$ or $\Delta l \sim q^{-1/3}$; (2) this range, Δl , is appreciably greater than one or two units in l ; and (3) the relevant l values are either all larger than $1/\theta$, so that $P_l(\cos \theta)$ is in the oscillatory regime or all smaller than $1/\theta$, so that the Bessel function representation of $P_l(\cos \theta)$ is good. To say that there must be very many phase shifts substantial in comparison with one radian to justify the semiclassical approximation is evidently only an imperfect simplification of the actual requirements.

The methods of analysis described here are applied in the following paper to some representative examples. There, from the potential and classical deflection function, one can evaluate the differential cross section; or, knowing the cross section, can work back to find the phase shift and classical deflection function. This information about the phase shift will allow one (7) to find part or all of the curve of potential, $V(r)$, as a function of distance.

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