UNIFORMLY APPROXIMATE SOLUTIONS FOR

SHORT-WAVE PROBLEMS

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ABSTRACT

The propagation of extremely short waves can be described entirely in terms of rays, and does not involve such concepts as wavelength or interference. When the waves are not so short, the simplest approximation consists in assigning to each ray system a complex exponential wave function with a phase proportional to the Hamilton-Jacobi function, and an amplitude proportional to the density of rays. But the true short-wavelength asymptotic form of wave-functions is non-uniform with respect to position variables, and this causes the simple approximation to diverge under certain circumstances.

There we examine a variety of physically interesting wave problems, and elicit the following general principle: the *uniformly* approximate asymptotic short-wavelength wave functions still involve the functions of ray theory, but the Hamilton-Jacobi functions now appear as the arguments of higher functions instead of in exponentials.

CONTENTS

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1. Introduction: the idea of a uniform approximation.

It often happens that, during the solution of some problem involving the diffraction and scattering of waves, one runs up against a wave function that cannot be evaluated in simple closed form in terms of the tabulated function of classical analysis. The quantity in question may be an integral, or the sum of a series, or the solution of a differential equation. The computer is no panacea in this connection: while it is always possible in principle to use a numerical method, it is actually often rather difficult to devise one that converges without proving something of the analytical behaviour of the function.

For waves which are extremely short in comparison with typical dimensions of scattering objects we do not need a wave theory at all - we can use geometrical optics for light, or classical mechanics in the case of matter. One can, in fact, set up a general axiomatic geometrical theory of rays and wave-fronts along the lines of the Hamilton-Jacobi theory of mechanics, without ever introducing such concepts as "wavelength" or "periodicity" (for a lucid account see Synge 1963). It is when the wavelength is short but not negligible that the problems can really start to get messy. The scattering of light by a raindrop, atoms from molecules, and high energy α- particles from nuclei, are related problems in this category; we shall meet many others. The most general statement of the standard procedure for dealing with such cases is the Geometrical theory of diffraction of Keller (1958) in which each ray system is assigned a sinusoidal or complex exponential wave function whose amplitude at a point ($\underline{r}$, t) is proportional to the square root of the density of rays at the point, and whose phase is the classical action or eikonal function of the ray system, measured in units so chosen that the wave function has the right periodicity; the total wave field is then the superposition of interfering contributions from the separate rays through the point in question. These results follow from an asymptotic solution of the wave equation (Born and Wolf 1959, P.108; Dirac 1947, P.121). When applied to quantum-mechanical problems, this geometrical theory of diffraction is called the WKB method (Wentzel 1926, Kramers 1926, Brillouin 1926).

This "semiclassical" procedure involving rays is simple enough in principle, but unfortunately, in all except the most trivial problems, it breaks down, since there are nearly always regions where the density of paths is infinite. Focal points and lines, and caustic surfaces in optics, or, in mechanics, surfaces where a beam of particles is reflected from a high potential, are examples of such anomalous regions. A re-examination of the derivation of the semi-classical wave-function shows that in fact it is not valid near such critical regions. Even if the wave function is not required in the critical region itself, there still remains the problem of using the semiclassical formula for a ray passing through the critical region. The phase function there may change rapidly (discontinuously, in the extreme short wave limit). In optics the best-known example of this is the phase advance by π on passage through a focus, resulting for instance in a dark fringe where one would expect the field to be bright in Meslin's interference experiment with a split lens (Feather 1960, P.218). In quantum mechanics the problem of the "connection formulae" between the probability amplitudes on both sides of a classical turning point is another example (see ~~Fumy~~ Furry 1946, Keller 1958).

Suppose, though, that one really does want the wave function in the critical region. It is possible to derive "transitional approximations" valid in and very near to the critical region, by finding the wave function actually at the critical point or line or surface and expanding outwards from there in a Taylor series; this is the basis of the "boundary layer" technique of Keller and Buchal (1959). However, this method has the disadvantage that it does not match smoothly on to the semiclassical ray solution outside the region.

In a growing number of cases these problems associated with critical regions have been solved by techniques of uniform approximation. These give analytic formulae valid near to or far from critical points. The appearance of the results leads us to formulate what we believe to be a new principle in wave theory. Under short wave conditions, uniform approximations to wave functions involve only quantities characterising the rays or paths of the corresponding geometrical or classical problem. The action functions of these paths, however, do not generally appear as variables in exponentials; instead, they are the arguments of higher transcendental functions which are characteristic of the geometrical form of the concentration of rays in the critical region. Thus, for instance, a simple caustic or single classical turning point can be described with the aid of an Airy function; an axial caustic needs the zero-order Bessel function; and a situation involving two classical turning points can be characterized by parabolic cylinder functions. FAr from the critical region the functions can be replaced by their known asymptotic approximations; these are exponential in form, so that the ray formulae are regained complete with the correct connections between opposite sides of the critical point.

Historically, the first uniform approximation was derived by Langer (1937) for the case of a single turning point in quantum mechanics; this required the use of the Airy function. It is interesting that Airy (1838) needed to define this function when calculating the first transitional approximation, in the theory of the rainbow (the most striking instance in nature of a ~~single~~ simple caustic). The method used by Langer of mapping the required solution of a differential equation onto the known solution of a simpler equation was generalized by Miller and Good (1953) and Dingle (1955). The analogous pioneering work for integrals was done by Chester, Friedman and Ursell (1957); their technique, an extension of the method of stationary phase, was applied by Berry (1966) to rainbow scattering, and by Ludwig (1966) to a more general treatment of wave functions near a caustic of any type.

In this report uniform approximations are derived for a variety of physical situations. Themethods used all involve a mapping of one variable on another. First, in § 2, an expression is derived for the water level during the passage of a tidal wave, this is a good introductory example, since it involves a simple special case of the method of Chester, Friedman and Ursell. In § 3 the generalized mapping method for differential equations is applied to derive new expressions for the scattering length in potential theory; the results depend in an interesting way on the precise form of the long-range tail of the scattering potential. Next, in § 4, a general semi classical theory of the scattering by a spherical disturbance is developed. This leads, in § 5 and § 6, to the first complete descriptions of rainbow and glory scattering. This last case involves the uniform approximation of a double integral. In § 7, an approximation is devised for the integral describing the de Haas van Alphen effect for an hour-glass-shaped Fermi surface. Finally, in § 8, we examine the modulation of light beams on passing through a time-dependent medium; this example is one of the very few which have no critical regions, so that the simple geometrical theory of diffraction provides a uniform approximation.

2. Tidal waves.

When an earthquake or explosion causes a local disturbance on the surface of the ocean, the propagation of the resulting wave is determined by the dispersive properties of water. These tidal waves or "tsunamis" are usually only about one foot high at most, but they travel extremely fast over very great distances, and are capable of causing great damage (Russell and Macmillan 1952, P.301). For simplicity, we consider one-dimensional waves (thus, for example, we might be considering the propagation of a pulse in a channel); certain complications arising in the two-dimensional case have not yet been fully resolved. We take the initial disturbance of the water surface y (x,t) as a stationary delta-function:

$$y(x,0) = A\,\delta(x) = \frac{A}{2\pi}\int_{-\infty}^{\infty} e^{ikx}\,dx$$

$$\dot{y}(x,0) = 0. \tag{1}$$

Each Fourier component propagates as a plane wave, and to satisfy the second boundary condition we need to take forward and backward-travelling waves equally. Thus

$$y(x,t) = \frac{A}{2\pi}\,\mathrm{Re}\int_{-\infty}^{\infty} e^{i(kx-\omega(k)t)}\,dk \tag{2}$$

$$= \frac{A}{2\pi}\,\mathrm{Re}\int_{0}^{\infty}\left[e^{i(kx-\omega(k)t)} + e^{-i(kx+\omega(k)t)}\right]dk. \tag{3}$$

For water waves on an ocean of depth h the dispersion relation is (Synge 1963)

$$\omega(k) = \sqrt{g\,k\,\tanh(hk)}\,. \tag{4}$$

This is an odd, analytic function of k.

It is not possible to evaluate (3) exactly in terms of standard functions, so we need an approximate method. This is not as disappointing as it seems: it would be pointless to calculate the value of (3) carefully for small x or t, since our delta function initial conditions is certainly unphysical. We have also omitted a surface tension term in (4). This corresponds to very large k not present in any actual initial disturbance; such short waves would be quickly attenuated anyway. The large t condition means that the ~~integral d~~ integrand is a very rapidly oscillating function of k; by the usual Kelvin stationary-phase arguments this implies that only certain regions of the path of integration give a contribution that is not cancelled by some other part.

The regions of k that we expect to contribute are those for which the phase is stationary; these satisfy

$$\frac{x}{t} = \frac{\partial \omega}{\partial k}(k)$$

$$\frac{x}{t} = -\frac{\partial \omega(k)}{\partial k}, \qquad (5)$$

for the two terms in (3) respectively. Figs. 1 and 2 are graphs of ω (k) and $\frac{\partial \omega(k)}{\partial k}$. Because $\frac{\partial \omega}{\partial k}(k)$ is even and positive the second integrand has no stationary points, and we shall ignore it from now on.

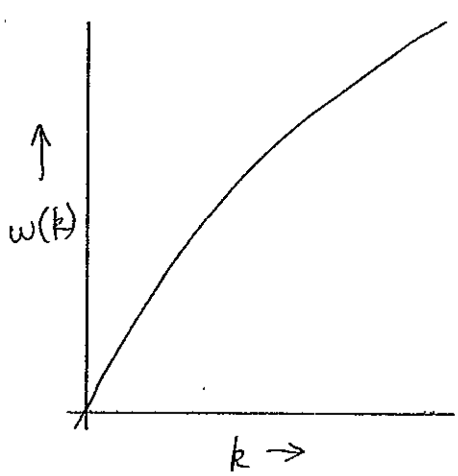

fig.1 Dispersion relation for water waves

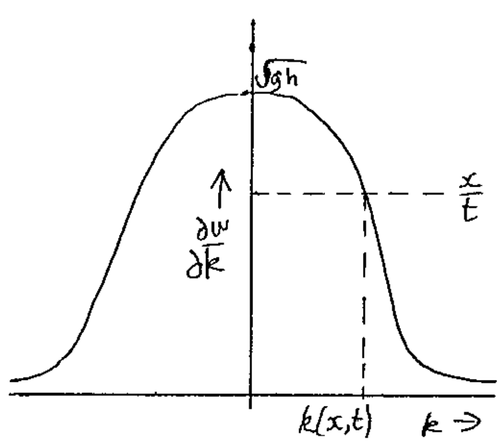

fig.2. Group velocity for water waves

The contribution of a given k to the integral propagates with the <u>group velocity</u> $v_g = \frac{\partial \omega}{\partial k}(k)$. The significant aspect of the present problem is that this has a maximum value, $\sqrt{gh}$, for waves long compared with the depth.

It is convenient to consider the state of the wave for different x at a fixed large t . If $x \gg t\sqrt{gh}$ there is no possible k that can contribute to the integral - the wave has not yet reached such distant points. We expect the front of the disturbance to propagate with the maximum group velocity, $\sqrt{gh}$. If $0 \ll x \ll t\sqrt{gh}$ the contributing group corresponds to waves of local wave number $k(x,t)$, and the conventional method of stationary phase (Copson 1965) can be applied for the first integral in (3), giving

$$y(x,t) \simeq \frac{A}{\sqrt{2\pi t\left|\frac{\partial^2\omega(k(x,t))}{\partial k^2}\right|}}\cos\left[k(x,t)x - \omega(k(x,t))t + \frac{\pi}{4}\right] \qquad (0 \ll x \ll t\sqrt{gh})$$

$$\simeq 0 \qquad (x \gg t\sqrt{gh}) \,. \qquad (6)$$

This result shows that locally, the motion consists of a quasi-sinusoidal train of waves with a length $2\pi/(k(x,t))$ which changes slowly from place to place (Havelock 1914).

It is interesting to interpret this motion in Hamiltonian terms (Eckart 1948). We envisage the asymptotic propagation as the motion of particles - "hydrons" (see Synge 1963) - whose dynamics is specified in terms of the conjugate position x and momentum k by the Hamiltonian function $\omega\,(x,k)$. Hamilton's ~~first~~ equations ~~is~~ are

$$\dot{k} = -\frac{\partial\omega}{\partial x} = 0$$

so that k = constant,

and $\dot{x} = \frac{\partial\omega(k)}{\partial k}$ = constant.

Thus a hydron moves with constant speed $\dot{x}$ and momentum k, but the larger its momentum, the slower it goes (see fig. 2); the fastest hydrons move with speed $\sqrt{gh}$ and have no momentum at all ! The Hamilton-Jacobi phase function $S\,(x,t)$ satisfies

$$\omega\left(\frac{\partial S}{\partial x}(x,t)\right) = -\frac{\partial S}{\partial t}$$

with the boundary condition $S\,(0,0)=0$, corresponding to the emission of a burst of particles from the origin at $t = 0$. A solution of this equation is

$$S_K(x,t) = Kx - \omega(K)t,$$

which involves the arbitrary constant K. We must eliminate this if we want Hamilton's Principal function for propagation between (0 0) and (x,t) that is, we must choose K such that

$$\frac{\partial S}{\partial K} = 0 = x - \frac{\partial\omega}{\partial K}(K).$$

But the K thus defined is identical with our $k\,(x,t)$, and the resulting function

$$S(x,t) = k(x,t)x - \omega(k(x,t))t$$

is identical with the phase of the wave group (6). It is zero for $x = \sqrt{gh}\,t$ and negative if $x < \sqrt{gh}\,t$. (The function $S_K(x,t)$ corresponds to a continuous stream of hydrons with fixed momentum K, and is analogous to our plane wave $e^{ikx - \omega(k)t}$.)

So far we have derived the semiclassical result, equation (6). As we go farther from the origin, the contributing waves get longer and longer (fig.2) until at $x = \sqrt{gh}\, t$ the group would appear to consist of waves of infinite length. As this happens, however, the value of $\frac{\partial^2\omega}{\partial k^2}$ decreases to zero (fig.3), and the result (6) diverges

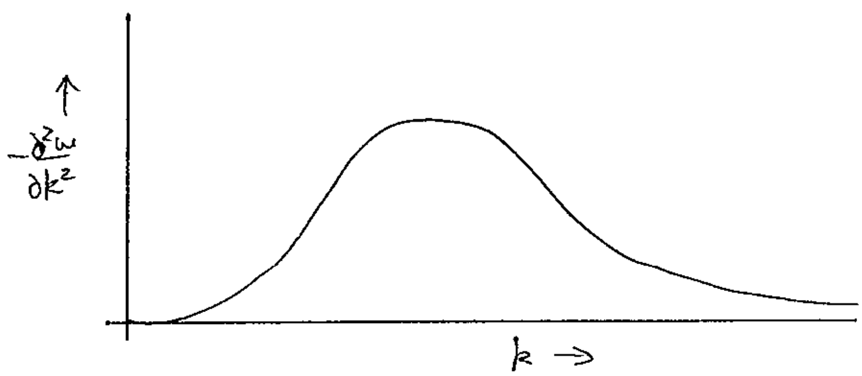

Fig 3. Rate of change of group velocity with k.

What we want is a uniform approximation which will give the value of $y(x,t)$ in the physically interesting region near the front of the wave, as well as describing the decay beyond the front and reducing to (6) behind it.

In the conventional method of stationary phase, used to derive (6) from (3), the phase of the exponent was expanded about $k = k(x,t)$, giving

$$kx - \omega(k)t = k(x,t)x - \omega(k(x,t))t - \frac{[k - k(x,t)]^2}{2}\frac{\partial^2\omega(k(x,t))t}{\partial k^2} + \text{higher terms.} \qquad (7)$$

The first order term in $k - k(x,t)$ is zero on account of (5). Near $k = 0$ the quadratic term becomes smaller than the cubic, and we must modify our expansion to allow for this. We could, of course, simply expand about $k = 0$, and write

$$kx - \omega(k)t = \left[x - \frac{\partial\omega}{\partial k}(0)t\right]k - \frac{k^3}{6}\frac{\partial^3\omega(0)}{\partial k^3}t + \cdots \tag{8}$$

where we have retained the linear term since we are no longer expanding about the stationary point. This would yield acceptable results very close to the wave front - in fact it would give the transitional expansion - but it is of no use for the main body of the wave, since it contains no reference to the stationary points.

What we do to get a uniform approximation is to map k onto a new integration variable X by means of the substitution

$$kx - \omega(k)t = -B(x,t)X + X^3/3, \tag{9}$$

(Chester et al 1957) in which the end $k = 0$ of the integration corresponds with $X = 0$. For the mapping to be one-to-one, we must choose $B(x,t)$ in such a way that dk/dX is never zero or infinite. But

$$\left(x - \frac{\partial\omega}{\partial k}t\right)\frac{dk}{dX} = -B(x,t) + X^2 \tag{10}$$

so we must make the point $X = (B(x,t))^{1/2}$ correspond with $k = k(x,t)$. This is very important, since it means that the stationary points of the new and old integrals correspond. We can find $B(x,t)$ by substituting in (9):

$$k(x,t)x - \omega(k(x,t))t = S(x,t) = -\frac{2}{3}\left[B(x,t)\right]^{3/2}, \tag{11}$$

or

$$B(x,t) = \left[-\frac{3}{2}S(x,t)\right]^{2/3}. \tag{12}$$

The first integral in (3) can now be transformed into

$$y(x,t) = \frac{A}{2\pi}\,\mathrm{Re}\int_0^\infty f(X)\, e^{i\left(-BX + \frac{X^3}{3}\right)}\, dX, \tag{13}$$

where $$f(X) = \frac{dk}{dX} \tag{14}$$

~~where~~ and we have taken ∞ for the upper limit of x on the grounds that its precise value is immaterial since the integral converges by virtue of its rapid oscillations long before this limit is reached.

So far our transformation is merely formal; the art in deriving a uniform approximation lies in the way we expand $f(X)$. What we do is to realise that the value of the integral arises principally from the immediate neighbourhood of the stationary point, so we write $f(X)$ as

$$f(X) = C + (X^2 - B)\, g(X) \tag{15}$$

(We use $X^2 - B$ rather than $X - B^{1/2}$ since $f(X)$ is an even function).

If $g(X)$ is regular, the second term vanishes at the critical point so we expect the integral to be well approximated if we just write

$$f(X) = C = f\left((B(x,t))^{1/2} \right)$$

To evaluate this we need $\frac{dk}{dX}(k(x,t))$, and we can get it by differentiating (10); this gives

$$\left(x - \frac{\partial \omega}{\partial k} t\right) \frac{d^2 k}{dX^2} - \frac{\partial^2 \omega}{\partial k^2} t \left(\frac{dk}{dX}\right)^2 = 2X, \tag{16}$$

or, at the point $X = B^{1/2}$,

$$C = \frac{dk}{dX}(X = B^{1/2}) = \left(\frac{2B^{1/2}}{-t \frac{\partial^2 \omega(k(x,t))}{\partial k^2}} \right)^{1/2} \tag{17}$$

Provided C is real, substitution in (13) gives

$$\boxed{y(x,t) = \frac{A\, B^{1/4}(x,t)}{\left(-2t \frac{\partial^2 \omega(k(x,t))}{\partial k^2}\right)^{1/2}} Ai\left(-B(x,t)\right)} \tag{18}$$

as our uniform approximation, where $Ai(z)$ is the Airy function (see Abramowitz and Stegun 1964).

Let us now examine this solution to see how it behaves in the three regions of interest. First we consider the main body of the wave, where $x \ll \sqrt{gh}\,t$. Then the phase $S(x,t)$ (see (ii)) is large and negative, so that $\beta(x,t)$ (see (12)) is large and positive. The Airy function then has a large negative argument, and we can use the appropriate asymptotic form

$$Ai(-|z|) \doteq \frac{1}{\sqrt{\pi}\,|z|^{1/4}} \sin\left[\frac{2}{3}|z|^{3/2} + \frac{\pi}{4}\right], \tag{19}$$

so that the water level becomes

$$y(x,t) = \frac{A}{\sqrt{-2i\,\frac{\partial^2\omega}{\partial k^2}(k(x,t))}} \sin\left(-S(x,t) + \pi/4\right)$$

which is identical with our semiclassical result (6).

Now let us see how the wave decays beyond the front, when $x \gg \sqrt{gh}\,t$. The first equation in (5) now has no real roots k (for $x \ll \sqrt{gh}\,t$ it had two, at $\pm k(x,t)$ and we ignored the negative one when deriving (6) since it was not on the path of integration). But $\partial\omega/\partial k$ is an even analytic function, so it is real on the imaginary k-axis $k = ik_y$ (see fig.4), where it increases from $\sqrt{gh}$.

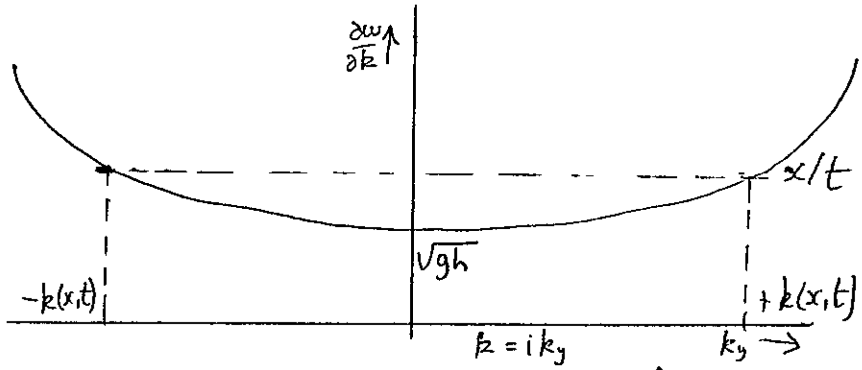

fig (5) group velocity for imaginary "momentum" k .

The appropriate solution of (5) is therefore one of the two purely imaginary roots $k = e^{\pm i\pi/2}|k(x,t)|$; of these we must take that root for which the coefficient $B(x,t)$ in the mapping (9) is real. But B is given by (12), so we must examine the phase S along the real axis; being an odd function, ω is purely imaginary along $k = ik_y$ as shown in fig. 6.

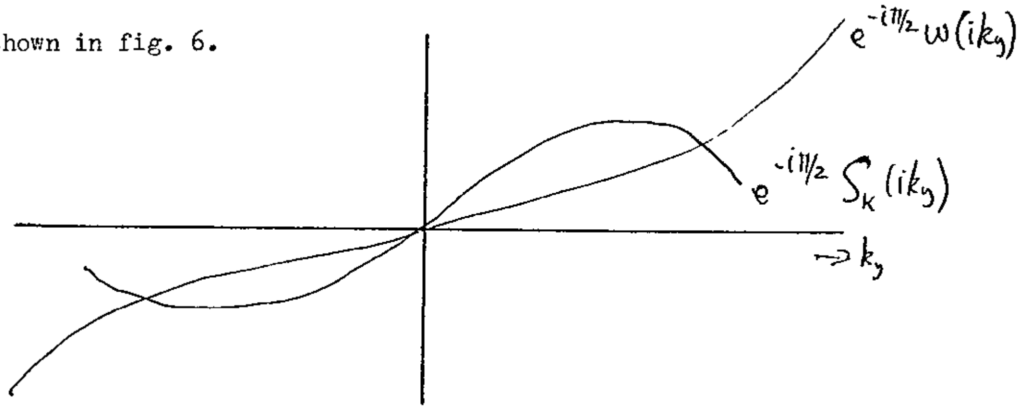

Fig. 6. dispersion relation and phase for imaginary k .

For the two roots, then, we have

$$k(x,t) = e^{\pm i\pi/2}|k|,$$

$$S(x,t) = e^{\pm i\pi/2}|S|,$$

$$B(x,t) = \left(\tfrac{3}{2}e^{i\pi}e^{\pm i\pi/2}|S|\right)^{2/3} = |B|e^{i\pi} \text{ or } |B|e^{i\pi/3},$$

provided we interpret the-sign in (12) as $e^{+i\pi}$. We must therefore take the root $k = e^{+i\pi/2}|k|$ if we want to keep B real. The second derivative $\frac{\partial^2\omega}{\partial k^2}$ that occurs in the expression (17) for C is negative imaginary for this root, so when $x > \sqrt{gh}\,t$

$$C = \left[\frac{2\left(e^{i\pi}|B|\right)^{1/2}}{(-)(-)\,e^{i\pi/2}\left|\frac{\partial^2\omega}{\partial k^2}\right|t}\right]^{1/2} = \left(\frac{2|B|^{1/2}}{t\left|\frac{\partial^2\omega}{\partial k^2}\right|}\right)^{1/2} = \text{real positive}$$

Our evaluation of the "real part" in the integral (13) is thus justified. If we had taken the-sign in (12) as $e^{-i\pi}$ we would have had to take the root $k = e^{-i\pi/2}|k|$; $\frac{\partial^2\omega}{\partial k^2}$ would have been positive imaginary and C would still have been positive real. After these analytic subtleties we can now evaluate our result (18) for $x \gg \sqrt{gh}\,t$ using the asymptotic form of the Airy function valid for large positive argument, namely

$$Ai(|z|) \approx \frac{e^{-\frac{2}{3}|z|^{3/2}}}{2\sqrt{\pi}\;|z|^{1/4}}, \tag{20}$$

The result is that the decaying wave form far beyond the front takes the form

$$y(x,t) = \frac{A}{2}\sqrt{\frac{1}{2\pi t\left|\frac{\partial^2\omega}{\partial k^2}(k(x,t))\right|}}\; e^{-|S(x,t)|} \,. \tag{21}$$

This result is a rather complicated instance of the association of a complex wave-number with an evanescent disturbance; a simple example occurs immediately outside a medium in which a wave has been totally reflected.

Now let us look at the immediate neighbourhood of the front - let us derive the transitional approximation (Jeffreys and Jeffreys 1962, P.517). We need the expansion for small k of the dispersion formula (4). This is

$$\omega(k) \approx \sqrt{gh}\,k - \sqrt{gh}\,\frac{h^2k^3}{6},$$

so that

$$\frac{\partial\omega}{\partial k} \approx \sqrt{gh} - \sqrt{gh}\,\frac{h^2k^2}{2}$$

and

$$\frac{\partial^2\omega}{\partial k^2} \approx -\sqrt{gh}\,h^2k$$

Then thw wave number of the contributing group is

$$k(x,t) = \left[\left(\sqrt{gh} - \frac{x}{t}\right)\frac{2}{h^2\sqrt{gh}}\right]^{1/2}.$$

The phase function is

$$S(x,t) = k(x,t)\,x - \omega\big(k(x,t)\big)t$$

$$= -\frac{2\sqrt{2}}{3}\left(\sqrt{gh} - \frac{x}{t}\right)^{3/2} \frac{t}{h\,(gh)^{1/4}} \, .$$

The argument of the Airy function is thus

$$-B(x,t) = -\left(-\tfrac{3}{2}\,S(x,t)\right)^{2/3} = \frac{x - \sqrt{gh}\,t}{\left(\frac{t}{2}\,g^{1/2}\,h^{5/2}\right)^{1/3}}$$

The function C multiplying the Airy function is

$$C = \left[\frac{2B^{1/2}}{-\frac{\partial^2\omega}{\partial k^2}\,t}\right]^{1/2}$$

$$= \left(\frac{2}{t\,g^{1/2}\,h^{5/2}}\right)^{1/3}$$

This is finite, unlike the $\left(\frac{\partial^2\omega}{\partial k^2}\right)^{-1/2}$ which causes (6) to diverge. Thus, in the transition region, substitution in (18) shows that

$$y(x,t) \approx \frac{A}{2\left(\frac{h^{5/2}g^{1/2}t}{2}\right)^{1/3}}\, Ai\left[\frac{x - \sqrt{gh}\,t}{\left(\frac{h^{5/2}g^{1/2}t}{2}\right)^{1/3}}\right] . \tag{22}$$

The general character of the wave is now clear: very far from the source the water surface is undisturbed. As we pass through the front at $x = t\sqrt{gh}$, the elevation shows the characteristic oscillations of the Airy function. Far behind the front the amplitude of the oscillations dies away, reflecting the increase of $\partial^2\omega/\partial k^2$ with k (see fig. 3; the eventual decrease for large k affects the behaviour only for small x where our methods are not valid).

The second crest of the wave occurs where the value of the argument, $-B$, of the Airy function, is about -5; if the transitional approximation is still valid there, (22) shows that the "wavelength" - the distance between the first and second crests is about

$$\Lambda = 4\left(h^{5/2} g^{1/2} t/2\right)^{1/3}$$
$$= \left(32\, x h^2\right)^{1/3}$$

(we must remember that the first crest is not quite at B = 0 but near B = 1). If, as in the pacific, $h \sim 5\,km$ and $x \sim 7 \times 10^3\,km$ (Tokyo to San Francisco), then

$$\Lambda \sim (32 \times 7 \times 25)^{1/3} \times 10$$
$$\sim 170\,km .$$

3. Scattering lengths; the tails of potentials and bound states.

In the quantum theory of the scattering of particles of mass m and energy E by a potential $V(r)$, one has to solve the radial schrodinger equation

$$\left.\begin{aligned} &\frac{d^2}{dr^2}\chi_\ell(r) + \left[\frac{2m}{\hbar^2}\left(E - V(r)\right) - \frac{\ell(\ell+1)}{r^2}\right]\chi_\ell(r) = 0 \\ &\chi_\ell(0) = 0 \end{aligned}\right\} \qquad (23)$$

The asymptotic form of the solution gives the phase shifts, η_ℓ since

$$\chi_\ell(r) \xrightarrow[r \to \infty]{} A \sin\left(kr - \frac{\ell\pi}{2} + \eta_\ell\right),$$
$$\text{where} \quad E = \hbar^2 k^2 / 2m . \qquad (24)$$

Of particular interest in nuclear and metal physics is the scattering at low energies. Then only the S-wave matters, and the wave function (24) takes the limiting form

$$\underset{k=0}{\chi_0(r)} = A \sin\eta_0 \left(1 + r \lim_{k \to 0} k \cot\eta_0\right)$$
$$= A \sin\eta_0 \left(1 - \frac{r}{a}\right). \qquad (25)$$

The quantity

$$a = -\lim_{k\to 0}\left(\frac{1}{k\cot\eta_0}\right) \tag{26}$$

is known as the scattering length, and it is shown in the standard works on scattering theory (e.g. Mott and Massey 1965, P.43) that it exists for all potentials that fall off faster than r^{-3} at large r. The significance of a lies in the fact that the low-energy limit of the total scattering cross-section is

$$Q = 4\pi a^2$$

The scattering length also determines, approximately, the position of the bottom of the conduction band in metals (Ziman 1967).

If we can solve the schrödinger equation (23) for $\ell = E = 0$, we can use our knowledge of the asymptotic form (25) to read off the scattering length. It turns out that a method for the uniform approximation of the solutions of differential equations, devised by Miller and Good (1953) and Dingle (1955), is ideally suited for this problem. We shall be interested in finding the functional dependence of the scattering length on the strength of the potential for cases where the tail of the potential takes various different forms. First of all, however, let us examine the relationship between the behaviour we expect to find and the s-wave bound states, if any, of the potential (we only consider attractive potentials).

In (24) the phase shift η_0 appears modulo π. Let us define a "complete phase shift".

$$\eta_0 = n\pi + \delta_0 \ , \text{ where } \ 0 \leq \delta < \pi .$$

Then n is the excess number of nodes, between the origin and a fixed large value of r, that the radial wave function $\chi_0(r)$ posesses as compared with the free wave function $\sin kr$ (the origin is not counted as a node). Fig. 7 shows an example where $n = 2$.

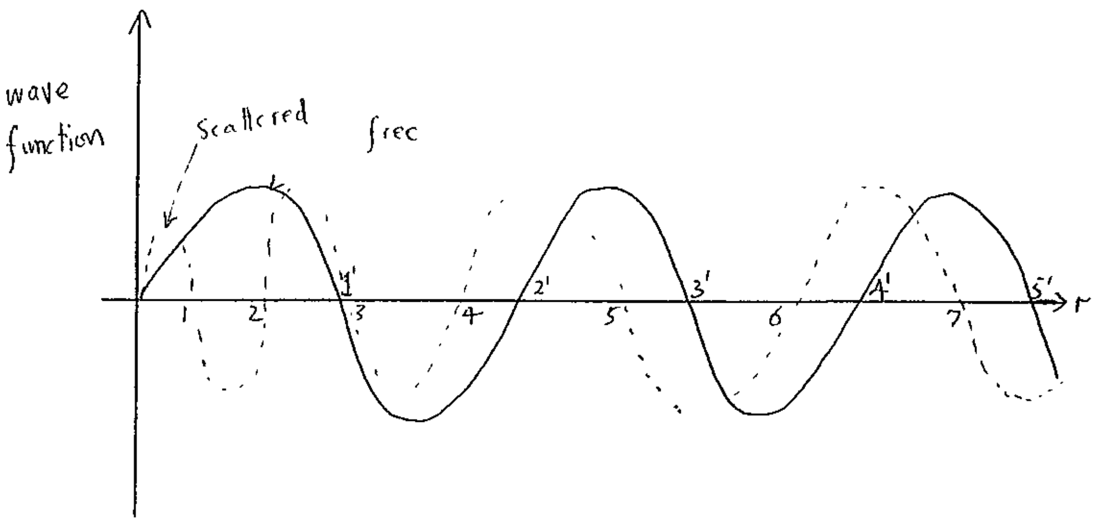

Fig.7. definition of complete phase shift

When $k \to 0$, δ_0 tends to zero proportionally to k (this is what makes the scattering length a constant), but η_0 can still be an integral number of π's ; this corresponds to residual nodes at $k = 0$ (see fig.8, for a case where $\eta_0 = 5\pi$)

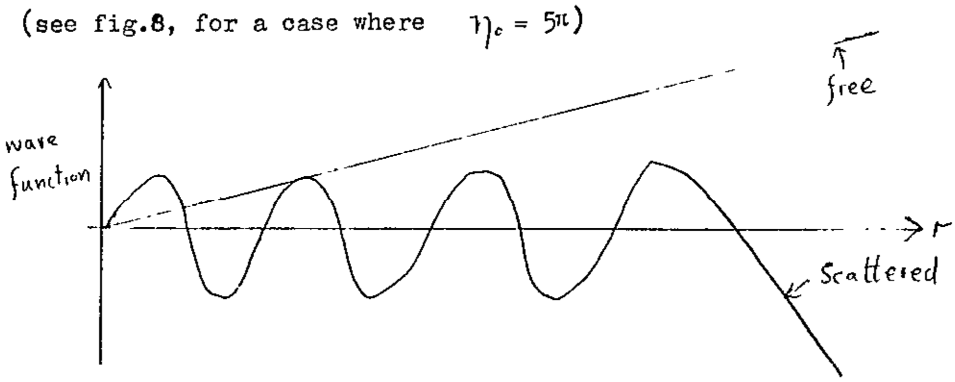

Fig.8. Wave function at $k = 0$.

Now let us consider the situation at negative energies. Unless one happens to choose a bound state energy, the wave function is exponentially divergent, with a number of nodes equal to the number of bound states below that energy. This means that if a given $V(r)$ has n bound states, the wave function at $k = 0$ has just n nodes. This result, that $\eta_0 = n\pi$ for a potential with n bound states, is called Levinson's theorem (Mott and Massey 1965, p.156). (The infinite number of nodes above $E = 0$ corresponds to the infinite density of states in the continuum.

Now imagine that we gradually increase the strength of the potential (say by altering some parameter in it) in such a way that the number of bound states changes from n to $n+1$ —— we suck down a state from the continuum. The $k = 0$ wave function then changes in a sequence illustrated in fig.9. This shows that, as the bound state squeezes through $k = 0$, the asymptotic slope of the wave

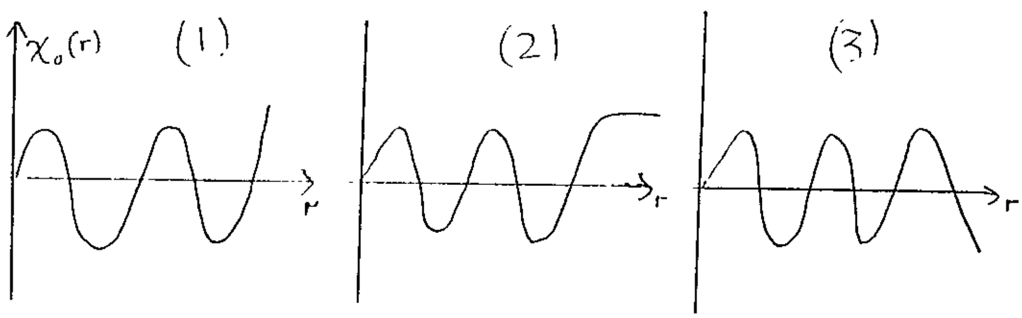

Fig.9. change in wave function as bound state passes through $k = 0$.

function becomes zero, and the scattering length becomes infinite. Let us now examine this analytically. We define the positive quantity

$$U(r) = -\frac{2m}{\hbar^2} V(r)$$

for our attractive potential, so that we have to solve

$$\left.\begin{aligned} \frac{d^2\chi_0}{dr^2} + U(r)\chi_0 &= 0 \\ \chi_0(0) &= 0 \end{aligned}\right\} . \tag{27}$$

Let us map the solution of this equation on to the known solution of an equation

$$\frac{d^2\psi}{d\sigma^2} + W(\sigma)\psi = 0, \tag{28}$$

(Miller & Good, 1953, Dingle, 1955), where the function W is in some sense similar to U — in our case we have to choose a W that goes to zero for large argument in a similar manner to U. We write our unknown function in terms of the known ψ in the form

$$\chi_0(r) = \left(\frac{d\sigma(r)}{dr}\right)^{-1/2} \psi(\sigma(r)), \tag{29}$$

where ψ is chosen so that χ satisfies the boundary conditions; our problem is thus reduced to finding the mapping function $\sigma(r)$.
Simple differentiation and use of (27) and (28) gives

$$U(r) = \left(\frac{d\sigma(r)}{dr}\right)^2 W(\sigma) - \left(\frac{d\sigma}{dr}\right)^{1/2} \frac{d^2}{dr^2}\left(\frac{d\sigma}{dr}\right)^{-1/2}.$$

Now if we have chosen W sufficiently similar in analytic behaviour to U we expect $\sigma(r)$ to be nearly proportional to r, so $\frac{d\sigma}{dr}$ is nearly constant; we thus expect the second term to be negligible compared with the first, so that, approximately,

$$\frac{d\sigma}{dr} = \left(\frac{U}{W}\right)^{1/2} \tag{30}$$

As our implicit equation for σ we therefore have

$$\int_{\sigma}^{b} \sqrt{W(\sigma)}\, d\sigma = \int_{r}^{a} \sqrt{U(r)}\, dr \equiv \phi(r). \tag{31}$$

It is necessary to take the respective zeros a and b of $U(r)$ and ~~with~~ $W(\sigma)$ as the upper limits of integration, so that $r = a$ corresponds with $\sigma = b$; if we did not do this (30) would be zero or infinite and we would not have a regular mapping. In our problem a and b are infinite for analytic potentials and finite for cut-off, "muffin-tin" potentials. Our general approximate solution is therefore

$$\chi_c(r) = \left(\frac{W(\sigma(r))}{U(r)}\right)^{1/4} \psi(\sigma(r)), \tag{32}$$

We now treat several different types of potential.

(i) Discontinuous cut-off at $r = R$.

This type of potential is shown in fig. 10, together with a suitable comparison $W(\sigma)$. This particular case of a constant comparison function just gives the results of the simple WKB method in quantum mechanics (Kemble 1958, P. 90).

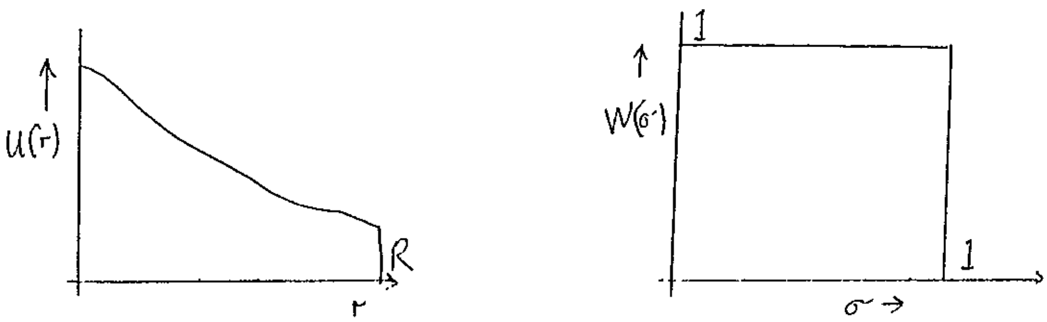

Fig. 10 Discontinuous cut-off potential and comparison function.

For the region $0 < \sigma < 1$ we have, from (28)

$$\psi(\sigma) = \alpha \sin(\sigma + \beta)$$

and from (30)

$$\int_{\sigma(r)}^{1} 1\, d\sigma = 1 - \sigma(r) = \int_{r}^{R} \sqrt{U(r)}\, dr = \phi(r),$$

so that (32) becomes

$$\chi_0(r) \approx \frac{\alpha}{[U(r)]^{1/4}} \sin\left(\beta + 1 - \phi(r)\right).$$

The boundary condition at $r = 0$ gives $\beta + 1 = \phi(0)$, so that

$$\chi_0(r) = \frac{-\alpha}{[U(r)]^{1/4}} \sin\left(\phi(r) - \phi(0)\right).$$

We must match this in slope and value at $r = R$ with the known solution (25) valid for $r > R$. This gives

$$\frac{\alpha}{[U(R)]^{1/4}} \sin \phi(0) = A \sin \eta_0 \left(1 - \frac{R}{a}\right),$$

and

$$\alpha\left[U(R)\right]^{1/4}\cos\phi(0) = -\frac{A\sin\eta_0}{a}$$

We have not differentiated the $\left[U(r)\right]^{-1/4}$ since this came from the $\left(\frac{d\sigma'}{dr}\right)^{-1/2}$ that we assumed was nearly constant in the argument leading to (30). More exactly, we assumed that dU/dr is small compared with $4U^{3/2}(R)$, which is true if the potential is fairly slowly-varying near the cut-off. The result for the scattering length is

$$\boxed{a = -\frac{\tan\phi(0)}{\sqrt{U(R)}} + R} \tag{33}$$

This shows that the "strength" of the potential can be characterised by the integral

$$\phi(0) = \int_0^\infty \sqrt{-\frac{2m}{\hbar^2}V(r)}\,dr, \tag{34}$$

which is just the Hamilton-Jacobi phase function for the propagation of particles of zero energy from the centre of the scatterer out radially to infinity. When its value passes through $(n+\frac{1}{2})\pi$, a becomes infinite. This indicates the passage through E = 0 of a bound state; the nearest integer below $\frac{\phi(0)}{\pi}+\frac{1}{2}$ gives the number of bound states in the potential. The passage of a through zero is the Ramsauer-Townsend effect (see Mott and Massey, 1965, P.31). Fig.11 shows how a varies with $\phi(0)$ for constant discontinuity $U(R)$.

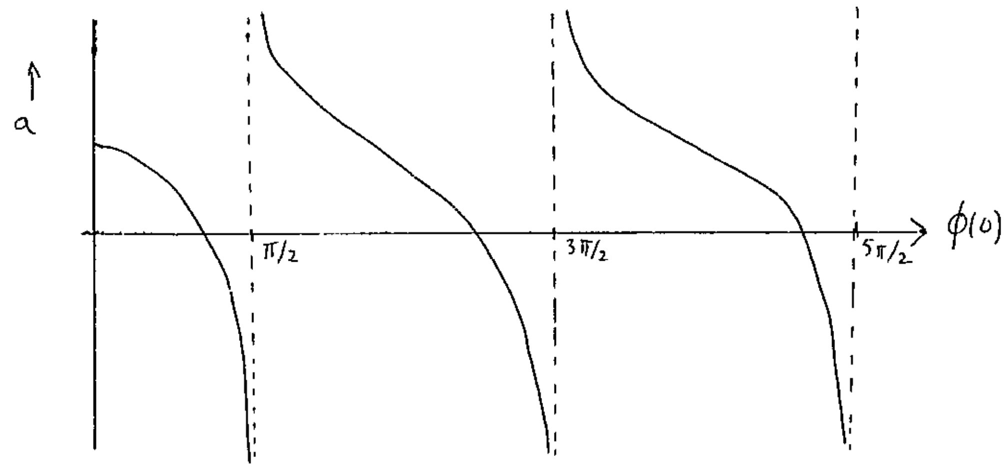

Fig.11 variation of scattering length with strength of potential

The curve is imphysical near $\phi = 0$ since it would imply a $\mathcal{U}$ of the form $A\delta(r - R)$, which is too quickly varying for our method to be valid. In fact to characterise a weak potential we would need R small too.

(ii) Discontinuity at $r = R$ in slope or higher derivative.

The formula (33) and the method leading to it break down if $\mathcal{U}(R) = 0$; this occurs when, to take an example from solid state physics, an atomic potential is "muffin-tinned" by taking the lattice zero of energy at some negative value with respect to that of the free atom (fig.12)

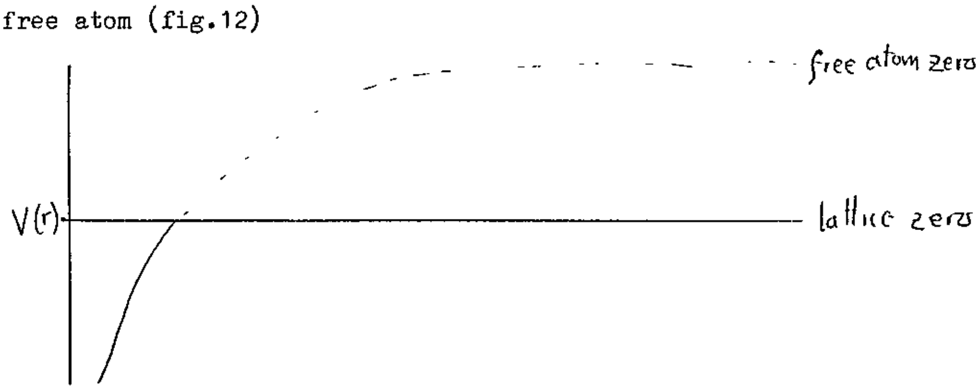

Fig.12 genesis of muffin-fin potential

In order to treat this analytically, we choose a comparison function $W(\sigma)$, which has a discontinuity of slope but not value at $\sigma' = \sigma$ (fig.13)

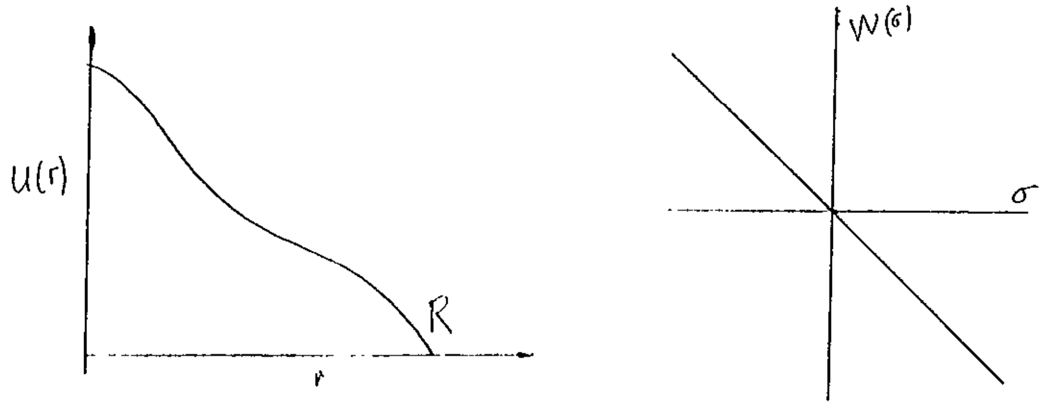

Fig.13. Comparison function and potential for case of slope discontinuity.

In the region $\sigma < 0$ then, we have, as our comparison equation

$$\frac{d^2\psi}{d\sigma^2} - \sigma\psi = 0,$$

so that (Abramowitz-~~Estegin,~~ Stegun 1964 , P.446)

$$\psi(\sigma) = \alpha\left(Ai(\sigma) + \beta Bi(\sigma)\right),$$

where, from (31)

$$\int_{\sigma}^{0} (-\sigma)^{1/2}\, d\sigma = \int_{r}^{R} \sqrt{U(r)}\, dr = \phi(r),$$

so that

$$\sigma(r) = -\left(\tfrac{3}{2}\phi(r)\right)^{2/3}.$$

Our approximate wave function is thus

$$\chi_0(r) \simeq \alpha\left[\frac{\left(\frac{3}{2}\phi(r)\right)^{2/3}}{U(r)}\right]^{1/4}\left(Ai(\sigma) + \beta Bi(\sigma)\right). \qquad (35)$$

The point $r = 0$ corresponds to $\sigma = \sigma_0 = -\left(\frac{3}{2}\phi(0)\right)^{2/3}$, so

$$\beta = -\frac{Ai(\sigma_0)}{Bi(\sigma_0)}. \qquad (36)$$

At the cut-off $r = R$, σ is zero, and our first boundary condition linking (34) with (25) is

$$\alpha\left(\lim_{r\to R} \frac{-\sigma(r)}{U(r)}\right)^{1/4} \frac{1+\beta\sqrt{3}}{3^{2/3}\,\Gamma(2/3)} = A\sin\eta_0\left(1-\frac{R}{a}\right).$$

The matching of derivatives gives

$$-\alpha\left(\lim_{r\to R} \frac{-\sigma(r)}{U(r)}\right)^{1/4}\left(\lim_{r\to R}\frac{U(r)}{-\sigma(r)}\right)\frac{1-\beta\sqrt{3}}{3^{1/3}\,\Gamma(1/3)} = -\frac{A\sin\eta_0}{a}.$$

To evaluate the limit we realise that, near $r = R$, we can write

$$U(r) = \left(-U'(R)\right)(R-r) + \cdots ,$$

so that

$$\phi(r) = \int_r^R \sqrt{R-r}\,dr\sqrt{-U'(R)} = \frac{2}{3}(R-r)^{3/2}\sqrt{-U'(R)},$$

and

$$\sigma(r) = -\left(-U'(R)\right)^{1/3}(R-r),$$

giving

$$\lim_{r\to R}\frac{U(r)}{-\sigma(r)} = \left(-U'(R)\right)^{2/3}.$$

The scattering length is therefore given by

$$\boxed{a = \frac{\Gamma(1/3)/\Gamma(2/3)\left[Bi\left(-\left(\frac{3}{2}\phi(0)\right)^{2/3}\right)-\sqrt{3}\,Ai\left(-\left(\frac{3}{2}\phi(0)\right)^{2/3}\right)\right]}{3^{1/3}\left[-U'(R)\right]^{1/3}\left[Bi\left(-\left(\frac{3}{2}\phi(0)\right)^{2/3}\right)+\sqrt{3}\,Ai\left(-\left(\frac{3}{2}\phi(0)\right)^{2/3}\right)\right]} + R} \tag{37}$$

An interesting special case of this formula arises when there are more than one or two bound states, since then $\phi(0)$ is large enough for us to use the asymptotic forms of the Airy functions. The result of a short calculation is

$$\boxed{a \approx -\frac{1.37}{\left[-U'(R)\right]^{1/3}}\frac{\sin\left(\phi(0)+\frac{\pi}{12}\right)}{\cos\left(\phi(0)-\frac{\pi}{12}\right)} + R} \tag{38}$$

This is similar to (33), except that it diverges when ϕ passes through $(n+\frac{7}{12})\pi$.

It is of interest to give the results for the case where the lowest discontinuous derivation at $r = R$ is the n^{th}, $U^{(n)}(R)$. Then we take

$$W(\sigma) = (-)^n \sigma^n$$

and

$$\sigma(r) = -\left(\frac{n+2}{2}\left(\phi(r)\right)\right)^{\frac{2}{n+2}},$$

The comparison functions are

$$\psi(\sigma) = \alpha\left(-\sigma(r)\right)^{1/2}\left[J_{\frac{1}{n+2}}\left(\frac{2}{n+2}(-\sigma)^{\frac{n+2}{2}}\right) + \beta J_{\frac{-1}{n+2}}\left(\frac{2}{n+2}(-\sigma)^{\frac{n+2}{2}}\right)\right],$$

so that

$$\chi_0(r) = \alpha\left[\frac{(-\sigma)^n}{U(r)}\right]^{1/4}\left(-\sigma'(r)\right)^{1/2}\left[J_{\frac{1}{n+2}}\left(\phi(r)\right) + \beta J_{-\frac{1}{n+2}}\left(\phi(r)\right)\right].$$

The resulting value of the scattering length is

$$\boxed{a = -\frac{(n+2)^{-\frac{n}{n+2}}\,\Gamma\left(\frac{1}{n+2}\right)}{\Gamma\left(\frac{n+1}{n+2}\right)}\left[\frac{\lfloor n}{(-)^n U^{(n)}(R)}\right]^{\frac{1}{n+2}} \frac{J_{\frac{1}{n+2}}\left(\phi(0)\right)}{J_{-\frac{1}{n+2}}\left(\phi(0)\right)} + R\,.} \tag{39}$$

The previous formulae, (33) and (37), are contained in this general result; they correspond to taking $n = 0$ or 1. Where there are many bound states, the scattering length becomes

$$\boxed{a = -\frac{(n+2)^{-\frac{n}{n+2}}\,\Gamma\left(\frac{1}{n+2}\right)}{\Gamma\left(\frac{n+1}{n+2}\right)}\left[\frac{\lfloor n}{(-)^n U^{(n)}(R)}\right]^{\frac{1}{n+2}} \frac{\sin\left(\phi(0) + \frac{n\pi}{4(n+2)}\right)}{\cos\left(\phi(0) - \frac{n\pi}{4(n+2)}\right)} + R\,,} \tag{40}$$

which shows that bound states pass through, giving infinitely strong scattering, whenever ϕ passes through $(m+\frac{1}{2}+\frac{n}{4(n+2)})\pi$.

(iii) Inverse power-law decay of potential tail

If the potential does not go to zero discontinuously at a finite radius but decays as $-\alpha/(\gamma+r)^s$, we can take $W(\sigma) = 1/\sigma^s$ (fig.14) as our comparison potential.

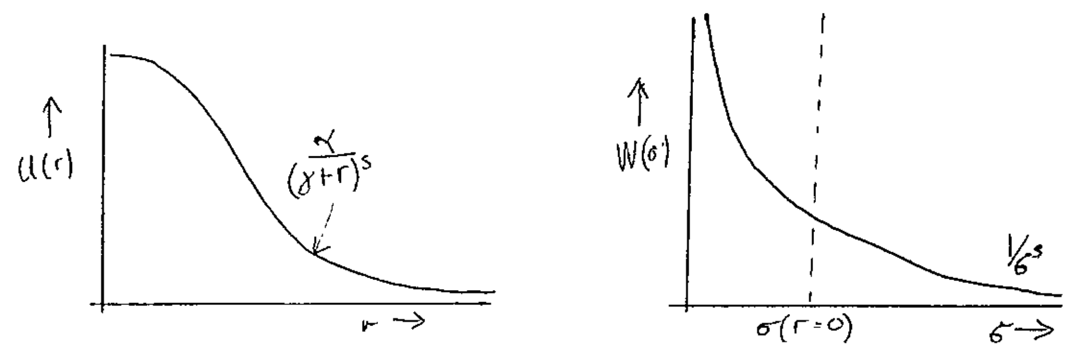

Fig.14. Comparison function and potential for inverse power-law decay

Then the points $\sigma' = \infty$ and $r = \infty$ correspond, so that (31) gives

$$\phi(r) = \int_{\sigma'}^{\infty} \sigma'^{-\frac{s}{2}}\, d\sigma = \frac{\sigma'^{-\frac{s}{2}+1}}{\frac{s}{2}-1}$$

It is easy to see from this example why we must make $W(\sigma)$ fall off asymptotically in the same way as $U(r)$. For if $U(r)$ behaved like, say, $\alpha/(\gamma+r)^t$ where $t \neq s$, then we should have

$$\frac{d\sigma}{dr} = \sqrt{\frac{U}{W}} \xrightarrow[r\to\infty]{} \frac{K\sigma'^{s}}{(r+\gamma)^t}$$

$$\propto \frac{(r+\gamma)^{(-\frac{t}{2}+1)(\frac{s}{-\frac{s}{2}+1})}}{(r+\gamma)^t} = (r+\gamma)^{\frac{t-s}{s-1}},$$

which goes to zero or infinity depending on whether $s \gtrless t$; the mapping would thus not be regular, and the reasoning leading up to (30) would break down.

The comparison equation is

$$\frac{d^2\psi}{d\sigma^2} + \sigma^{-s}\psi = 0 ,$$

which has the solution (Abramowitz & Stegun) 1964, p. 362)

$$\psi(\sigma) = \alpha\,\sigma^{1/2}\left[J_{\frac{1}{s-2}}\left(\frac{2\sigma^{1-s/2}}{s-2}\right) + \beta J_{\frac{-1}{s-2}}\left(\frac{2}{s-2}\sigma^{1-\frac{s}{2}}\right)\right]$$

$$\propto \left(\phi(r)\right)^{\frac{1}{2-s}}\left[J_{\frac{1}{s-2}}\left(\phi(r)\right) + \beta J_{\frac{-1}{s-2}}\left(\phi(r)\right)\right].$$

The boundary condition at the origin demands that we take

$$\beta = \frac{-J_{\frac{1}{s-2}}\left(\phi(0)\right)}{J_{\frac{-1}{s-2}}\left(\phi(0)\right)} . \tag{41}$$

Our approximate wave function is thus

$$\chi_0(r) = \left(\frac{W}{U}\right)^{1/4}\phi^{\frac{1}{2-s}}\left[J_{\frac{1}{s-2}}\left(\phi(r)\right) + \beta J_{\frac{-1}{s-2}}\left(\phi(r)\right)\right].$$

To get the scattering length we must expand this for large r ; this involves the Bessel functions of small argument; for $s > 3$ only the first two terms are non vanishing, and the wave function is thus

$$\chi_0(r) = C\left[\frac{1}{2^{\frac{1}{s-2}}\,\Gamma\left(1+\frac{1}{s-2}\right)} + \beta\frac{\phi^{-2/s-2}\,2^{1/s-2}}{\Gamma\left(1-\frac{1}{s-2}\right)}\right]$$

$$\propto\left[1 + \beta\frac{\Gamma\left(1+\frac{1}{s-2}\right)}{\Gamma\left(1-\frac{1}{s-2}\right)}\alpha^{-\frac{1}{s-2}}(r+\gamma)(s-2)^{2/s-2}\right],$$

If we compare this with (25), and use (41), we see that the scattering length is

$$\boxed{a = \frac{\Gamma\left(1-\frac{1}{s-2}\right)\alpha^{1/s-2}\,J_{-\frac{1}{s-2}}\left(\phi(0)\right)}{\Gamma\left(1+\frac{1}{s-2}\right)(s-2)^{2/s-2}\,J_{\frac{1}{s-2}}\left(\phi(0)\right)} - \gamma} . \tag{42}$$

For large ϕ (o), this result becomes

$$\boxed{a = \frac{\Gamma\left(1-\frac{1}{s-2}\right)\alpha^{1/s-2}\sin\left(\phi(0)+\frac{s\pi}{4(s-2)}\right)}{\Gamma\left(1+\frac{1}{s-2}\right)(s-2)^{2/s-2}\cos\left(\phi(0)-\frac{s\pi}{4(s-2)}\right)} - \gamma .} \tag{43}$$

An interesting check on the correctness of these formulae is provided by the fact that they can be derived from (39) or (40) by putting $R = -\gamma$, $n = -s$, $U^{(n)}/\underline{|n} = \alpha$, since the form of the potential near its vanishing point is then

$$U(r) = \frac{(r\;\;R)^n U^{(n)}}{\underline{|n}} = \frac{\alpha}{(r+\gamma)^s} .$$

(iv) <u>Exponentially decaying potential</u>

This final example cannot be derived from any of the previous formulae; if for example, we try to use the method of the last section, putting $S = \infty$, we run into trouble because J-o and J + o are not independent functions. We write

$$W(\sigma) = e^{-2\sigma} , \quad U(r) \underset{r\to\infty}{\longrightarrow} Ae^{-r/R} ,$$

so that

$$\int_\sigma^\infty e^{-\sigma} d\sigma = e^{-\sigma} = \phi(r) ,$$

$$\sigma = -\ln \phi(r) .$$

Our solution $\psi(\sigma)$ on to which we map our radial wave function is (Abramovitz & Stegun 1964,P.362)

$$\psi(\sigma) = \alpha\left(J_0(e^{-\sigma}) + \beta Y_0(e^{-\sigma})\right),$$

so that

$$\chi_0(r) \approx \left(\frac{W(\sigma)}{U(r)}\right)^{1/4} \alpha \left[J_0(\phi(r)) + \beta Y_0(\phi(r))\right] ,$$

where

$$\beta = -\frac{J_0(\phi(0))}{Y_0(\phi(0))} .$$

We must now expand this for large r , to enable us to identify the scattering length; when r is large, ϕ is small, having the form

$$\phi \to 2RA^{1/2} e^{-r/2R} .$$

The only surviving terms of the wave function are

$$\chi_0(r) \propto \left[1 + \frac{2\beta}{\pi} \left(\ln \frac{\phi(r)}{2} + \gamma \right) \right]$$

$$= 1 + \frac{2\beta}{\pi} \left(\gamma + \ln (RA^{1/2}) \right) - \frac{\beta}{\pi} \frac{r}{R} .$$

where γ is Euler's constant, $\gamma = .577216$. The scattering length is thus

$$\boxed{a = -\pi R \frac{Y_0(\phi(0))}{J_0(\phi(0))} + 2R\left(\gamma + \ln (RA^{1/2})\right)} \tag{44}$$

Comparison of this with (39) or its special cases (33) or (37) shows that this exponential potential is in some ways equivalent to a force with the finite range

$$R' = 2\gamma R + 2R \ln (RA^{1/2}).$$

The results we have derived in §§ (2.i) - (2.iv) each give the scattering length as an analytic functional of the potential. These functionals approximate uniformly in V (r) to the exact values of a , provided that the comparison function W (σ) is chosen so that $d\sigma(r)/dr$ is never zero or infinity when r is between 0 and ∞; this implies that W(σ) must fall to zero in the same way as V (r). The use of a uniform approximation to the radial wave function made it easy to satisfy the boundary condition at r = 0 and to find the asymptotic form for $r \to \infty$ which we needed to find a.

It is interesting to see how our results are related to the well-known Born approximation. All our formulae have involved (implicitly) the relation

$$a = \lim_{r \to \infty} \left(r - \frac{\chi_0(r)}{\chi_0'(r)} \right). \tag{45}$$

Now, when the potential is small we can take a small comparison function W (σ), and we can use the perturbation theory for $\psi(\sigma)$. We have

$$\psi''(\sigma) = -W(\sigma)\psi(\sigma).$$

The zeroth approximation is ψ_0 , where

$$\psi_0''(\sigma) = 0$$

so that

$$\psi_0(\sigma) = A\sigma + B$$
$$= A(\sigma - \sigma(0))$$

where $\sigma(0)$ is the point on the σ -axis corresponding to $r = 0$.
To a first-order approximation, $\psi = \psi_0 + \psi_1$, where

$$\psi_1''(\sigma) = -W(\sigma)\psi_0(\sigma),$$

The solution satisfying the boundary condition is

$$\psi_1(\sigma) = -A\int_{\sigma_0}^{\sigma} d\sigma_1 \int_{\sigma_0}^{\sigma_1} W(\sigma_2)(\sigma_2 - \sigma_0)\, d\sigma_2,$$

so that our comparison solution is

$$\psi(\sigma) = A\left(\sigma - \sigma_0 - \int_{\sigma_0}^{\sigma} d\sigma_1 \int_{\sigma_0}^{\sigma_1} W(\sigma_2)(\sigma_2 - \sigma_0)\, d\sigma_2\right)$$
$$= A\left(\sigma - \sigma(0) - \left[(\sigma_1 - \sigma_0)\int_{\sigma_0}^{\sigma_1} W(\sigma_2)(\sigma_2 - \sigma_0)\, d\sigma_2\right]_{\sigma_1 = \sigma} + \int_{\sigma_0}^{\sigma}(\sigma_1 - \sigma_0)^2 W(\sigma_1)\, d\sigma\right)$$
$$\xrightarrow[\sigma \to \infty]{} A\left[\sigma\left(1 - \int_{\sigma_0}^{\infty} W(\sigma)(\sigma - \sigma_0)\, d\sigma\right) + \int_{\sigma_0}^{\infty}(\sigma - \sigma_0)^2 W(\sigma)\, d\sigma - \sigma_0\left(1 - \int_{\sigma_0}^{\infty} W(\sigma)(\sigma - \sigma_0)\, d\sigma\right)\right].$$

Thus

$$\frac{\chi_0}{\chi_0'} \simeq \frac{1}{\frac{d\sigma}{dr}}\frac{\psi'}{\psi_0'} \sim \frac{1}{\frac{d\sigma}{dr}}\left(\sigma - \sigma_0 + \int_{\sigma_0}^{\infty}(\sigma - \sigma_0)^2 W(\sigma)\, d\sigma\right),$$

so that the scattering length is

$$a = \lim_{r \to \infty} \left(r - \frac{1}{\frac{d\sigma}{dr}} \left(\sigma - \sigma_0 + \int_{\sigma_0}^{\infty} (\sigma' - \sigma_0)^2 W(\sigma') \, d\sigma' \right) \right).$$

Now, when this formula is valid for small potentials we can write

$$\sigma - \sigma_0 \simeq \left(\frac{d\sigma}{dr} \right)_{\infty} r$$

This is because the smaller a potential is, the farther in from infinity does it have to be like its comparison function, for the approximation to hold uniformly. We can also change the integration variable from σ' to r, giving

$$\int_{\sigma_0}^{\infty} d\sigma' \, (\sigma' - \sigma_0)^2 \, W(\sigma')$$
$$= \int_0^{\infty} dr \, \frac{U(r)}{\left(\frac{d\sigma}{dr}\right)} \, r^2 \left(\frac{d\sigma}{dr} \right)^2_{r = \infty}$$
$$\simeq \left(\frac{d\sigma}{dr} \right)_{r = \infty} \int_0^{\infty} dr \, U(r) \, r^2$$

The final result for the scattering length is thus

$$\boxed{a \simeq \sqrt{\frac{2m}{\hbar^2}} \int_0^{\infty} V(r) \, r^2 \, dr} \qquad (46)$$

which is just the Born approximation (see Mott and Massey 1965, p.89).

Finally we emphasise that, unlike the Born approximation, all our formulae work well when there are any number of bound states. The asymptotic results also tell us that when the classical phase integral (measured in units of $\hbar$), given by

$$\phi = \frac{1}{\hbar} \sqrt{2m} \int_0^{\infty} \sqrt{-V(r)} \, dr,$$

increases through $(n + \frac{1}{2} + \varepsilon)\pi$, where ε is a phase constant which varies from 0 to $\pi/4$ according to the form of the potential tail, then the system gains its $(n+1)^{st}$ s-wave bound state, and the scattering length diverges.

4. Semiclassical scattering: the asymptotic formulation

The last section was concerned with aspects of the theory of scattering at very low energies, where only the s-wave is important. Now we shall investigate what happens at higher energies in the semiclassical case, where the de Broglie wavelength of the incident particles is small compared with the typical dimensions of the scatterer, so that many (hundreds or thousands) of partial waves contribute to the scattering. We shall concern ourselves with the angular distribution of the scattered radiation, characterised by the differential cross-section, whose exact expression is

$$\sigma(\theta) \equiv |f(\theta)|^2,$$

where,

$$f(\theta) = -i\left(\frac{\hbar^2}{2mE}\right)^{1/2} \sum_{l=0}^{\infty} \left(l+\tfrac{1}{2}\right)\left[e^{2i\eta_l} - 1\right] P_l(\cos\theta) \tag{47}$$

(see Mott and Massey 1965, Chap.2).

The numerical evaluation of this sum is not at all straightforward since under the conditions we envisage there are many terms with rapidly-varying phases. In the past there have been two main lines of approach. The first was motivated by the development of radio, with the consequent need to understand the propagation of waves round hard and penetrable uniform spheres. The pioneering work in this connection was done by Watson (1918) and Van der Pol and Bremmer (1937), who replaced the sum in (47) by a contour integral in the l-plane, which they then evaluated by the method of residues. The generalisation of these methods to cases where the potential is not a hard sphere or a square well was carried out by Regge (1957) (see Newton 1964, Nussenzweig 1965) this work has led to a great revival of interest in the analytic aspects of potential scattering, motivated primarily by the hope that it will lead to some understanding of elementary particles. If we are interested in actually getting at the value of the scattering amplitude, Regge pole techniques seem to be useful if the potential is either discontinuous or has a hard core.

For the smoother potentials which arise in the lower-energy quantum mechanics of collisions between atoms and molecules, a second, somewhat different, approach can be used. This was pioneered in two beautiful papers by Ford and Wheeler (1959), who replaced the sum in (47) by an integral over ℓ which they evaluated by the method of stationary phase deriving transitional approximations when this diverged. This work has been taken up and applied extensively to the results of experiments with molecular and atomic beams (Hundhausen and Pauly 1965, Mason and Monchick 1964, Munn and Smith 1966).

We shall follow this second approach, and work on or near the real positive ℓ-axis. The simple semiclassical result will diverge whenever the phase shifts η_ℓ takes certain forms; this gives rise to characteristic behaviour of $f(\theta)$ of which we shall treat <u>rainbow</u> and <u>glory scattering</u>. These terms are taken from analogous effects occurring in the scattering of sun light from raindrops (which of course represent a discontinuous potential and hence need Watson-Regge methods for their complete description). Our results will extend those of Ford and Wheeler by giving uniform approximations, valid over a wide range of angles.

We start by transforming the scattering amplitude from a sum to a series of integrals over ℓ by the Poisson sum formula (Lighthill 1958); it has been suggested by Pekeris (1950) that this is the natural mathematical tool to use when considering a mode or eigenfunction expansion in a region where ray or classical concepts are appropriate.

The result is

$$f(\theta) = -i\left(\frac{\hbar^2}{2mE}\right)^{1/2} \sum_{m=-\infty}^{\infty} e^{-im\pi} \int_0^{\infty} d\lambda\, \lambda \left[e^{2i\eta_{\lambda-\frac{1}{2}}} - 1\right] e^{2\pi i m\lambda}\, P_{\lambda-\frac{1}{2}}(\cos\theta), \tag{48}$$

where $\eta_{\lambda-\frac{1}{2}}$ and $P_{\lambda-\frac{1}{2}}(\cos\theta)$ are any convenient functions which reduce to η_ℓ and $P_\ell(\cos\theta)$ when $\lambda - \frac{1}{2}$ is integral. Later we shall see that there are familiar cases where it would be wrong to approximate this series by the term $m = 0$ (This would amount to replacing the sum in (47) by an integral, as Ford and Wheeler (1959)do); nevertheless, such cases are fairly rare, and, in general, only a few terms contribute, with more or less equal magnitude, the rest being negligible.

Under the semiclassical conditions we are dealing with, we require $\eta_{\lambda-\frac{1}{2}}$ and $P_{\lambda-\frac{1}{2}}(\cos\theta)$ to lowest order in $\hbar$. To do this consistently we must use the relation

$$L = \lambda\hbar, \tag{49}$$

giving the angular momentum in terms of the variable λ corresponding to the quantum number ℓ and then regard L as being of zero order in $\hbar$; this will only be justified if it turns out (as it does) that the scattering can be described using the values of L occurring if the same collision is treated classically. The lowest-order expression for the phase shift is then (Mott and Massey 1965, p.99)

$$\eta_{\lambda-\frac{1}{2}} = \frac{\tilde{\eta}(L)}{\hbar} + O(\hbar)\text{, where}$$

$$\tilde{\eta}(L) = (2mE)^{1/2}\left[\int_{r_0(L)}^{\infty}\left\{\left(1-\frac{V(r)}{E}-\frac{L^2}{2mEr^2}\right)^{1/2}-1\right\}dr - r_0(L)\right] + \frac{L\pi}{2}, \tag{50}$$

where $r_0(L)$ is the outermost zero of the square root. This means that

$$e^{2i\eta_{\lambda-\frac{1}{2}}} = e^{\frac{2i}{\hbar}\hat{\eta}(L)}\left(1 + O(\hbar)\right)$$

For the Legendre function the appropriate asymptotic form is (Szegö 1934)

$$P_{\lambda-\frac{1}{2}}(\cos\theta) \simeq \left(\frac{\theta}{\sin\theta}\right)^{1/2} J_0\left(\frac{L\theta}{\hbar}\right). \tag{51}$$

This is valid uniformly in θ for small $\hbar$, provided that $\theta < .828\pi$. Near π there is a similar formula involving $\pi - \theta$, which we can use if we want to treat scattering near the backward direction. With this proviso, the, we can insert these asymptotic forms for the phase shift and the Legendre function into our series of integrals for $f(\theta)$; this gives

$$f(\theta) = \frac{-i}{\hbar}\left(\frac{\theta}{2mE\sin\theta}\right)^{1/2} \sum_{m=-\infty}^{\infty} e^{-im\pi} \int_0^\infty dL\, L\, J_0\left(\frac{L\theta}{\hbar}\right) e^{\frac{2\pi i m L}{\hbar}} \times$$

$$\times \left(e^{\frac{2i\hat{\eta}(L)}{\hbar}} - 1\right). \tag{52}$$

In using the asymptotic forms right down to L = 0 we have assumed that the region of integration between 0 and a few units of $\hbar$ does not contribute to the integral.

We shall use this general formula (52) in § 6 when we consider glory scattering near $\theta \sim 0$; first however, we deal with scattering away from the forward direction. If $\theta \gg \frac{\hbar}{\text{smallest contributing } L}$, a condition which under semiclassical conditions holds down very small angles, we can replace the Bessel function in (5) by its asymptotic form for large argument. For non-forward angles we can also neglect the -1 term in (52) (this just subtracts the forward delta-function representing the incident wave); the scattering amplitude is then given by

$$f(\theta) = \frac{-i}{2(\pi\hbar m E \sin\theta)^{1/2}} \sum_{m=-\infty}^{\infty} e^{-im\pi} \left\{ e^{-\frac{i\pi}{4}} I_m^{+} + e^{+\frac{i\pi}{4}} I_m^{-} \right\},$$

where (53)

$$I_m^{\pm} = \int_0^{\infty} L^{1/2} e^{\frac{i}{\hbar}\left[2\tilde{\eta}(L) + L(\pm\theta + 2m\pi)\right]} dL. \tag{54}$$

These are the integrals we have to evaluate.

The integrands of $I_m^{\pm}$ are rapidly oscillating functions (because of the smallness of $\hbar$ in comparison with $2\tilde{\eta} + L(\pm\theta + 2m\pi)$ under quasi-classical conditions) and we therefore expect that, just as in §2 with the tidal waves, the main contributions to the integrals arise from stationary points on the positive real axis, whenever these exist. The stationary points in this case are those values of L which satisfy

$$\left.\begin{aligned} 2\frac{d\tilde{\eta}}{dL} &= \pi - \left(\frac{2}{mE}\right)^{1/2} L \int_0^{\infty} \frac{dr}{\left\{1 - \frac{V(r)}{E} - \frac{L^2}{2mEr^2}\right\}^{1/2}} \\ &\equiv \Theta(L) = \mp\theta - 2m\pi, \end{aligned}\right\} \tag{55}$$

where the upper and lower signs refer to I_m^{+} and I_m^{-} respectively. Following Ford and Wheeler (1959) we have here noted the quality of $2\,d\tilde{\eta}/dL$ with the classical deflection function $\Theta(L)$, which gives the <u>total</u> angle (positive for net repulsion, negative for net attraction) made with the forward direction by the classical paths of particles emerging after hitting the target with angular momentum L. Since $\Theta \leq +\pi$ (this is obvious from (55) as well as on dynamical grounds), the integrals $I_m^{\pm}$ for $m < 0$ have no stationary points on the path of integration and are thus negligible in comparison with any others which do have such points. This is precisely analogous to the absence of stationary points in the second integral (3) for the tidal wave problem. The particular one of the set of integrals (54) which contains the contribution of a given classical path depends, according to (55), on the manner in which the path encircles the target particle before emerging at the scattering angle θ.

Apart from the classical paths, which are solutions of (55) for real positive L, there are usually also stationary points off the real axis. These complex angular momenta, corresponding to 'complex classical paths', give exponentially small contributions to the integrals and, unless L is very close to the real axis, are negligible under quasi-classical conditions if there are any competing real paths. If there are no real paths, the scattering is very small depends entirely on the complex paths and is very difficult to calculate since it depends on the fine analytical details of the potential (see Patashinskii et al 1964 who use Regge methods for this case).

In the case of tidal waves we were dealing with coordinates x and t; here we have a steady state problem involving the constant energy E and coordinates r and Θ (the solutions we are interested in do not involve the azimuth ϕ). Nevertheless we can still give a Hamiltonian interpretation to what we have done. The Hamilton-Jacobi equation for the phase function $S(r, \theta)$ is

$$H(\underline{r}, \nabla S) = E$$

or

$$\frac{1}{2m}\left[\left(\frac{\partial S}{\partial r}\right)^2 + \frac{1}{r^2}\left(\frac{\partial S}{\partial \theta}\right)^2\right] + V(r) = E, \tag{56}$$

We can get a solution by separation of variables, in the form

$$S = S_1(\theta) + S_2(r)$$

If we write $\frac{\partial S}{\partial \theta} = -L = const$, then it is easy to show that the action is

$$S_L(r,\theta) = \int^r dr\sqrt{2mE\left(1 - \frac{V(r)}{E} - \frac{L^2}{2mr^2E}\right)} - L\theta + const \tag{57}$$

We are interested in particles that come from infinity and go to infinity, so we take the lower and upper limits of the integral to be both infinite, with the path of integration from ∞ to r_0, with the square root negative (corresponding to the radial momentum $p_r < 0$ for an incoming particle), then round the branch point at $r = r_0$ and out again to ∞ on the other side of the cut in the integrand where the square root is positive. Further, we choose the additive constant so that $S_L(r,\theta) = 0$ if there is no scattering potential - i.e. we refer the motion to that of a free particle. The result is

$$S_L(\theta) = 2\sqrt{2mE}\left[\int_{r_0}^{\infty}\left\{\left(1 - \frac{V(r)}{E} - \frac{L^2}{2mEr^2}\right)^{1/2} - 1\right\}dr - r_0(L)\right] + L(\pi - \theta). \tag{58}$$

If we interpret θ as the Θ of (55) - the total angle turned through, then $S_L(\Theta)$ is identical with the phase in the exponent of the integrals (54). This situation is precisely analogous to the case of the integral (3) for the tidal wave. There, the integration variable k was interpreted as the momentum conjugate to the variable of interest, x; here the variable L is the momentum conjugate to the angular coordinate θ.

Both k and L arose in the Hamiltonian treatments as separation constants in the Hamilton-Jacobi equation.

But (58) is not the solution we want, just as $kx - \omega(k)t$ was not the required phase in our tidal wave problems. Eq.(58) refers to a beam of particles with a single L, whereas our problem involves an incident plane wave containing all L. To get the correct solution we have to eliminate L, by the equation,

$$\frac{\partial S_L(\theta)}{\partial L} = 0.$$

This equation is identical with (55) and its solution(s) $L = L(\Theta)$ tell us which angular momenta correspond to particles deflected by Θ. The final result for the action ~~of~~ function at infinity for our scattered particles is thus

$$S(\Theta) = 2\tilde{\eta}\left(L(\Theta)\right) - L(\Theta)\Theta, \tag{59}$$

which is the analogue of $k(x,t)x - \omega(k(x,t))t$ in the tidal wave problem.

According to the philosophy guiding our methods of uniform approximation, we expect our final results for $f(\theta)$ to involve the phases $S(\Theta)$ along the contributing classical paths, even though these phases might not appear as the arguments of exponential functions; in §§ 5 and 6 we shall find that this is the case.

Before plunging into the details, it is interesting to digress and see what interpretation we can put on the integrals $I_m^{\pm}$ of (54). These give contributions to the scattering amplitude from all L, not just the $L(\theta)$ that appear classically. The phase of each contribution is the action $S_L(\theta)$ of (58); but we know very well that in general the classical path with a given L does not emerge at θ , so we are faced with the problem of finding just what motion it is that $S_L(\theta)$ describes. Now, our solution to the Hamilton-Jacobi equation has specified the angular momentum, but not the starting angle of the motion, so the set of paths we are dealing with is that shown (for a repulsive potential, in fig.15. The sphere $r = r_0$ is

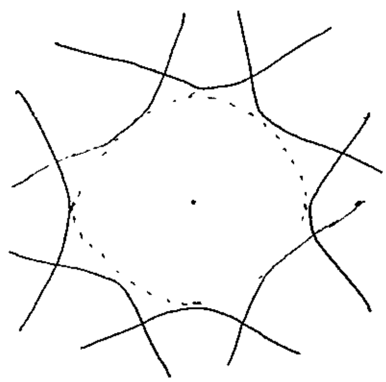

Fig.15 Classical paths with fixed angular momentum L

an envelope for these paths, so that, while motion on the surface of the sphere is not classical (in no sense does it correspond to a bound state) such motion may nevertheless be regarded as a singular solution of the Hamiltonian equations. If we accept such motions we can see how it is that a particle with a given angular momentum L can emerge at an arbitrary angle θ . Consider the situation shown in fig.16, where we are observing at an angle θ less than the angle θ_1 , at which the particle would normally emerge. We envisage the particle to travel in from infinity to r_0 and to travel round the sphere for an angular distance γ which is such that if it travels along a normal classical path after leaving it will emerge at θ . Let us call this a "pseudoclassical path"; what is the

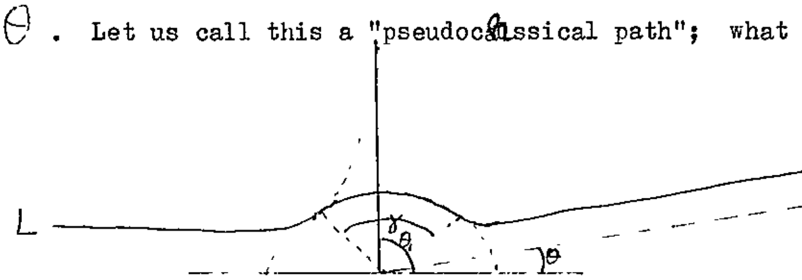

Fig.16. Pseudoclassical path enabling particle with L to emerge at θ .

action along it?

Along the two sections where $r > r_0$ the action is $2\tilde{\eta}(L) - L\theta_1$ while for the portion on the sphere it is $\int \underline{p} \cdot d\underline{r} = \int_{\theta}^{\theta+\gamma} p_\theta \, d\theta = L\gamma$. But simple geometry shows that $\gamma = \theta_1 - \theta$, so that the action along the whole pseudoclassical path, which is the sum of these two contributions, is exactly equal to $S_L(\theta)$ of (58). Fig. 17

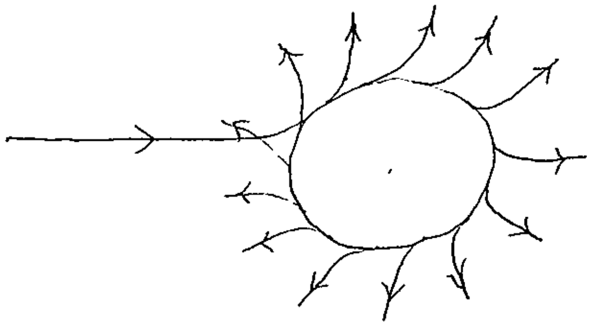

Fig.17. Set of pseudoclassical paths corresponding to action function $S_L(\theta)$.

shows the paths corresponding to this function.

A similar interpretation could be given to the two integrals (3) for the tidal wave problem, but it would not be so easy to visualise. There is, however, one important feature of the scattering situation that is not present in the tidal wave problem. If our pseudoclassical path does not emerge after traversing an angle γ on the sphere, but makes several circuits, traversing $\gamma + 2n\pi$ or if it traverses $\gamma + 2\theta + 2n\pi$ we shall still get a contribution at our observation angle θ ; these contributions from topologically different paths constitute the terms in the Poisson series (53). Only when L is an integral multiple of $\hbar$ will the contributions from successive circuits arrive at θ in phase; for other L the waves will interfere destructively. This then is the physical content of the Poisson sum formula; quantization arises when a point can be reached by an infinite number of topologically different routes. This has been noted before (Pekeris, Rubinow 1961), but the novelty of the present example arises because the paths are pseudoclassical.

Interesting though this line of thought is, it does not help us evaluate our integrals, since the different paths interfere destructively: if we sum all the pseudoclassical paths for the different circuits we just get back our scattering sum over integral ℓ, but if we integrate them for different L on the same circuit we get destructive interference except along our true classical paths, with $L(\theta)$ given by (55) and the phase by (59). We must remark, however, that these pseudoclassical paths seem to be the analogue for continuous potentials of the "creeping waves" which travel round the surfaces of hard scatterers, attenuating as they go (Keller 1958, Nussenzweig 1965). Of course creeping waves are much more important - they give contributions which do not cancel by interference, and are responsible for many of the useful properties of radio wave propagation.

5. Rainbow Scattering.

The way the scattering amplitude behaves as a function of θ depends on the number and nature of the stationary points of the integrals $I_m^{\pm}$. A function which displays this information in a useful way is $\Theta(L)$, defined in (55). This function is in every way equivalent to the group velocity $\frac{\partial\omega}{\partial k}$ (see fig.2). Stationary points occur, according to (55), at those values of L where $\Theta(L)$ takes one of the values $\pm\theta + 2n\pi$. The simplest form of deflection function which contains the rainbow and glory phenomena we wish to treat is shown in fig. 17a.

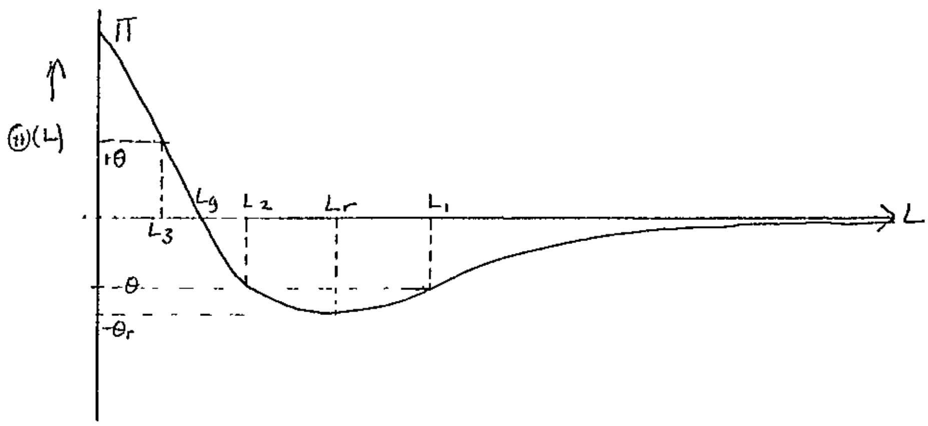

Fig.17a Typical deflection function for case of rainbow scattering.

A curve like this might arise,for example, in an intermolecular collision, where the potential is attractive at large distances and repulsive at short distances. The corresponding classical paths are shown in fig.18.

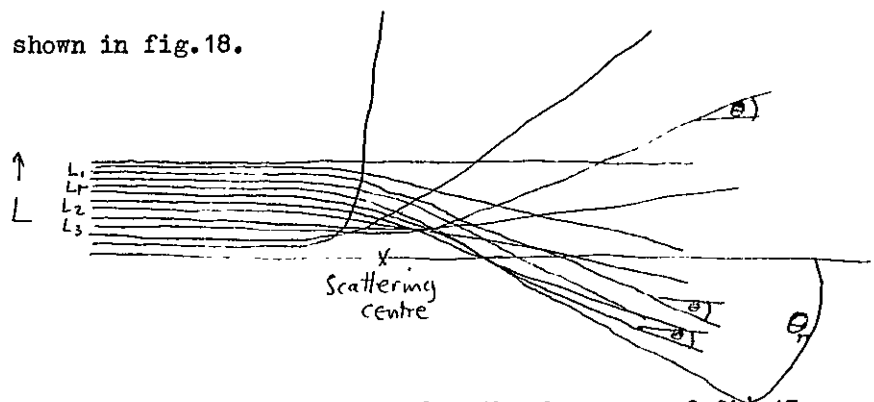

Fig.18. Sketch of classical paths for case of fig.17a

The important feature of this deflection function is that it has an extremum at $\Theta(L_r) = -\theta_r$; θ_r is called the rainbow angle. If $\theta < \theta_r$ there are three contributing paths, corresponding to stationary points at L_1 and L_2 for the integral I_0^+, and at L_3 for I_0^-. As θ increases through θ_r, L_1 and L_2 approach and coalesce, leaving only the contribution from L_3. It is this coalescence of stationary points that is responsible for the rainbow behaviour of $f(\theta)$; it can be seen from fig.18 that it is associated with a caustic of the system of classical paths. The whole problem of uniform expansions near caustics has recently been treated in a very general and rigorous way by Ludwig (1966).

It is a simple matter to write down the approximate value of $f(\theta)$ when θ is considerably less than the rainbow angle: we just apply the ordinary method of stationary phase (Copson 1964) to the two integrals I_0^+ and I_0^- - paying due regard to the signs of $\frac{d\Theta}{dL}$ - to get the results

$$\left.\begin{aligned} I_0^- &\simeq \sqrt{\frac{2\pi L_3(\theta)\hbar}{\left|\frac{d\Theta}{dL}(L_3(\theta))\right|}}\; e^{-\frac{i\pi}{4}}\; e^{\frac{i S_3(\theta)}{\hbar}} \\ I_0^+ &\simeq \sqrt{\frac{2\pi L_2(\theta)\hbar}{\left|\frac{d\Theta}{dL}(L_2(\theta))\right|}}\; e^{-\frac{i\pi}{4}}\; e^{\frac{i S_2(\theta)}{\hbar}} + \sqrt{\frac{2\pi L_1(\theta)\hbar}{\left|\frac{d\Theta}{dL}(L_1(\theta))\right|}}\; e^{+\frac{i\pi}{4}}\; e^{\frac{i S_1(\theta)}{\hbar}} \end{aligned}\right\} \qquad (60)$$

where S_n represents, in an obvious notation, the action (59) along the n^{th} contributing path. The scattering amplitude is thus given, by (53) as

$$f(\theta) = \frac{-i}{\sqrt{2mE\sin\theta}}\left[\sqrt{\frac{L_3(\theta)}{\left|\frac{d\Theta_3(\theta)}{dL}\right|}}\; e^{\frac{i S_3(\theta)}{\hbar}} + \sqrt{\frac{L_2(\theta)}{\left|\frac{d\Theta_2(\theta)}{dL}\right|}}\; e^{-\frac{i\pi}{2}}\; e^{\frac{i S_2(\theta)}{\hbar}} + \sqrt{\frac{L_1(\theta)}{\left|\frac{d\Theta_1(\theta)}{dL}\right|}}\; e^{\frac{i S_1(\theta)}{\hbar}}\right]. \qquad (61)$$

This is the typical semiclassical result with the the three rays contributing phase factors proportional to the action, and the additional phase difference of $\pi/2$ between 1 and 2 because of the caustic lying between them. As the classical limit is approached, the oscillations in $f(\theta)$ with angle or energy get faster and faster, until at last no instrument has sufficient resolution to detect them.

We then measure $\overline{|f(\theta)|^2}$, the mean being over several oscillations, and (61) gives

$$\overline{\sigma(\theta)} \to \frac{1}{2mE\sin\theta}\left[\frac{L_3(\theta)}{\left|\frac{d\Theta_3(\theta)}{dL}\right|} + \frac{L_2(\theta)}{\left|\frac{d\Theta_2(\theta)}{dL}\right|} + \frac{L_1(\theta)}{\left|\frac{d\Theta_1(\theta)}{dL}\right|}\right] \tag{62}$$

- the purely classical result, which does not involve $\hbar$.

When θ is in the general region of the rainbow angle the action differences $S_3 - S_2$ and $S_3 - S_1$ are much greater than $S_2 - S_1$ (S_3 corresponds physically to a different type of path corresponding to repulsion) so the oscillations between L_3 and the other two stationary points can be averaged away before that between L_1 and L_2, i.e. we can write

$$\sigma(\theta) = \frac{1}{2mE\sin\theta}\frac{L_3(\theta)}{\left|\frac{d\Theta_3(\theta)}{dL}\right|} + \left|\frac{I_0^+}{2\sqrt{\pi E\hbar m\sin\theta}}\right|^2$$

$$\equiv \frac{1}{2mE\sin\theta}\frac{L_3(\theta)}{\left|\frac{d\Theta_3(\theta)}{dL}\right|} + \sigma_r(\theta), \tag{63}$$

and isolate the rainbow behaviour which arises entirely from I_0^+.

So far we have considered $\theta \ll \theta_r$. At the other extreme, $\theta \gg \theta_r$, there are no real stationary points - no contributing rays (from I_0^+); instead there are two complex conjugate stationary points, giving an exponentially small contribution which can be neglected in comparison with that from the nonrainbow amplitude from L_3.

In the interesting region near θ_r, $\frac{d\Theta}{dL}$ is small and the approximation ~~58~~ (60) for I_0^+ diverges. This is precisely analogous to the breakdown of the Kelvin wave-group formula (6) at an extremum of the group velocity $\frac{d\omega}{dk}$. The method of dealing with this situation is similar to that used in § 2, except that the rainbow case is more complicated. The stationary points do not coalesce at one of the limits of integration, but both lie on the path of integration, and the integrand is not symmetrical about L_r.

We could, if we wished, derive a transitional approximation (Ford and Wheeler, 1959, Berry, 1966) valid if $\theta \approx \theta_r$, by expanding the phase in the integrand I_o^+ about the rainbow ray $L = L_r$, i.e. we could write

$$2\tilde{\eta}(L) + L\theta = 2\tilde{\eta}(L_r) + L_r\theta + \left(2\tilde{\eta}'(L_r) + \theta\right)(L - L_r) + $$
$$+ \quad 2\tilde{\eta}'''(L_r)\frac{(L-L_r)^3}{\lfloor 3}$$

substitute into (54) and evaluate the integral. But this is not a sufficiently flexible expansion to work far from θ_r since it contains no reference to the stationary points.

Just as in (9) we introduce a new integration variable X by the relation

$$2\tilde{\eta}(L) + L\theta = -\xi(\theta)X + \frac{X^3}{3} + A(\theta). \qquad \ldots .(64)$$

For the mapping to be one-to-one, $\frac{dL}{dX}$ must never be zero or infinite. But

$$\left(2\frac{d\tilde{\eta}}{dL} + \theta\right)\frac{dL}{dX} = -\xi(\theta) + X^2, \qquad \ldots .(65)$$

so that the stationary points of the two integrands must correspond, and we must have

$$X = +\xi^{1/2}(\theta) \longleftrightarrow L = L_1(\theta)$$
$$X = -\xi^{1/2}(\theta) \longleftrightarrow L = L_2(\theta). \qquad \ldots .(66)$$

When inserted into (65), these relations give

$$A(\theta) = \frac{1}{2}\left(S_1(\theta) + S_2(\theta)\right) \equiv \overline{S(\theta)} \qquad \ldots .(67)$$

and $$\frac{4}{3}\xi^{3/2} = S_2(\theta) - S_1(\theta) \equiv \Delta S(\theta) \qquad \ldots .(67)$$

involving the mean and difference of the actions along the two paths. In the classically lit region ($\theta < \theta_r$), L_1 and L_2 are both real, whereas in the shadow region they are complex conjugates. Thus $A(\theta)$ is always real. An examination of the phase relationships involved shows that we can always make ζ real, and that it is negative in the shadow region, where

$$\zeta_{\text{shadow}} = -\left(\frac{3}{2}\,\mathcal{I}_m\, S(\theta)\right)^{2/3} \qquad \ldots . (68)$$

($S(\theta)$ is the action along either path), and positive in the lit region where

$$\zeta_{lit} = +\left(\frac{3}{4}\,\Delta S(\theta)\right)^{2/3}. \qquad \ldots . (69)$$

The integral I_0^+ then becomes

$$I_0^+ = e^{i\frac{\bar{S}(\theta)}{\hbar}} \int_{-\infty}^{\infty} L(X)^{1/2}\frac{dL(X)}{dX}\, e^{\frac{i}{\hbar}\left(-\zeta X + \frac{X^3}{3}\right)} dX, \qquad \ldots . (70)$$

where the limits can be taken as written because only the region near the stationary points, now at $X = \pm\zeta^{\frac{1}{2}}$, is considered to contribute significantly to the integral.

The way in which the factor

$$f(X) = L^{\frac{1}{2}}\frac{dL}{dX}$$

in the integrand can be expanded to give an asymptotic expansion for the integral has been described by Chester et al (1957) and Ludwig and Bleistein (1966). To get the first term we write

$$f(X) = p + qX + (X^2 - \zeta)\,g(X). \qquad \ldots . (71)$$

Then, provided $g(X)$ is regular, the term $(X^2 - \zeta)g$ is zero at the important stationary points, so we are justified in just retaining $p + qX$. The qX term is necessary because the integrand is not symmetric about $X = 0$ as it was in the tidal wave example. The integra~~nd~~tion in (70) can now be done, to give

$$I_0^+ \simeq 2\pi\, e^{i\frac{\bar{S}(\theta)}{\hbar}}\left[\hbar^{1/3} p\, Ai\left(\frac{-\zeta}{\hbar^{2/3}}\right) - i\hbar^{2/3} q\, Ai'\left(\frac{-\zeta}{\hbar^{2/3}}\right)\right]. \qquad \ldots . (72)$$

To get p and q we introduce the relations (66) into the expansion (71), to obtain

$$f(\zeta^{1/2}) = p + q\zeta^{1/2}$$
$$f(-\zeta^{1/2}) = p - q\zeta^{1/2},$$

or

$$p = \frac{1}{2}\left[L_1^{1/2}\left(\frac{dL}{dX}\right)_{L_1} + L_2^{1/2}\left(\frac{dL}{dX}\right)_{L_2}\right]$$

$$q = \frac{1}{2\zeta^{1/2}}\left[L_1^{1/2}\left(\frac{dL}{dX}\right)_{L_1} - L_2^{1/2}\left(\frac{dL}{dX}\right)_{L_2}\right]. \qquad \ldots . (73)$$

The values of the derivatives $\frac{dL}{dX}$ at the two stationary points may be found by differentiating the relation (65) with respect to X; this gives

$$\Theta'\left(\frac{dL}{dX}\right)^2 + \left(\bar{\Theta} + \theta\right)\frac{dL}{dX} = 2X.$$

But the second term of this vanishes at the stationary points, and we have

$$\left(\frac{dL}{dX}\right)_{L_1} = \left(\frac{2\zeta^{1/2}}{\Theta'(L_1)}\right)^{1/2}$$

$$\left(\frac{dL}{dX}\right)_{L_2} = \left(\frac{2\zeta^{1/2}}{-\Theta'(L_2)}\right)^{1/2}, \qquad \ldots . (74)$$

By inserting (74) into (73), and (73) into (72) we finally obtain the uniform approximation to the rainbow integral I_0^+ :

$$\boxed{I_0^+ = \pi\sqrt{2}\, e^{i\frac{S(\zeta)}{\hbar}}\left\{\left[\left(\frac{L_1}{\Theta'(L_1)}\right)^{1/2} + \left(\frac{L_2}{-\Theta'(L_2)}\right)^{1/2}\right]\frac{\zeta^{1/4}}{\hbar^{-1/3}} Ai\left(-\frac{\zeta}{\hbar^{2/3}}\right) + \bar{Q}i\left[\left(\frac{L_1}{\Theta'(L_1)}\right)^{1/2} - \left(\frac{L_2}{-\Theta'(L_2)}\right)^{1/2}\right]\frac{\zeta^{-1/4}}{\hbar^{-2/3}} Ai'\left(-\frac{\zeta}{\hbar^{2/3}}\right)\right\}} \qquad \ldots . (75)$$

In the lit region, $(\theta < \theta_r)$, where $\zeta > 0$, the rainbow cross-section is

$$\boxed{\sigma_r(\theta) = \frac{\pi}{2mE\sin\theta}\left\{\left[\left(\frac{L_1}{\Theta'(L_1)}\right)^{1/2} + \left(\frac{L_2}{|\Theta'(L_2)|}\right)^{1/2}\right]^2 \frac{\zeta^{1/2}}{\hbar^{1/3}} Ai^2\left(-\frac{\zeta}{\hbar^{2/3}}\right) + \left[\left(\frac{L_1}{\Theta'(L_1)}\right)^{1/2} - \left(\frac{L_2}{|\Theta'(L_2)|}\right)^{1/2}\right]^2 \frac{\hbar^{1/3}}{\zeta^{1/2}} Ai'^2\left(-\frac{\zeta}{\hbar^{2/3}}\right)\right\}} \qquad \ldots . (76)$$

Far from Θ_r the difference in action between the two contributing paths is many units of $\hbar$; hence ζ is large and we may replace the Airy functions by their asymptotic forms (19 and (20). The two terms of (75) are then both of zero order in $\hbar$, and their sum reduces exactly to the semiclassical result (60).

On the dark side of the rainbow we have

$$L_{\substack{1\\2}}(\theta) = |L(\theta)|\, e^{\pm i\alpha(\theta)}$$

$$\Theta'_{\substack{1\\2}}(\theta) = |\Theta(\theta)|\, e^{\pm i\beta(\theta)}.$$

If these expressions are used in (75), the resulting rainbow cross-section is

$$\boxed{\begin{aligned}\sigma_r(\theta) = \frac{\pi |L(\theta)|}{mE\sin\theta|\Theta'(\theta)|}\Big\{&\Big[1-\sin(\alpha(\theta)-\beta(\theta))\Big]\frac{|\zeta|^{1/2}}{\hbar^{1/3}}\,Ai^2\Big(\frac{|\zeta|}{\hbar^{2/3}}\Big)+\\ &+\Big[1+\sin(\alpha(\theta)-\beta(\theta))\Big]\frac{\hbar^{1/3}}{|\zeta|^{1/2}}\,Ai'^2\Big(\frac{|\zeta|}{\hbar^{2/3}}\Big)\Big\}\end{aligned}} \quad \ldots (77)$$

To get the transitional approximation from (75) we evaluate the various quantities using the expansion about the rainbow ray (just before eq.(64). L_1 and L_2 are given by

$$2\tilde{\eta}(L_r) + \theta + \tilde{\eta}'''(L_r)(L-L_r)^2 = 0,$$

$$L_{\substack{1\\2}} \approx L_r \pm \sqrt{\frac{\theta_r - \theta}{\tilde{\eta}'''(L_r)}}$$

since $\quad 2\tilde{\eta}'(L_r) = \Theta \quad$ from (55). Also,

$$S_{\substack{1\\2}}(\theta) \doteq 2\tilde{\eta}(L_r) + L_r\theta \mp \frac{2}{3}\frac{(\theta_r-\theta)^{3/2}}{(\tilde{\eta}'''(L_r))^{1/2}},$$

so that

$$\overline{S(\theta)} = 2\tilde{\eta}(L_r) + L_r\theta$$

and

$$\zeta = \frac{\theta_r - \theta}{(\tilde{\eta}'''(L_r))^{1/3}}.$$

Finally,

$$\Theta'(L_{\frac{1}{2}}) \simeq 2\tilde{\eta}'''(L_r)(L_{\frac{1}{2}} - L_r) = \pm 2\sqrt{\tilde{\eta}'''(L_r)(\theta_r - \theta)} \,.$$

If we insert all these quantities into (75), omitting the term in Ai' since for small ζ (near the rainbow edge) it is of order $\hbar^{2/3}$ relative to the term in Ai, we get

$$I_0^+ \approx \frac{2\pi L_r^{1/2}\hbar^{1/2}}{\left[\tilde{\eta}'''(L_r)\right]^{1/3}} e^{\frac{i}{\hbar}\left[2\tilde{\eta}(L_r) + L_r\theta\right]} Ai\left[\frac{\theta - \theta_r}{\left(\hbar^2\tilde{\eta}'''(L_r)\right)^{1/3}}\right] \qquad \dots . (78)$$

so that

$$\sigma_r(\theta) = \frac{\pi L_r \, Ai^2\left[(\theta - \theta_r)/\{\hbar^2\eta'''(L_r)\}^{1/3}\right]}{\hbar^{2/3} m E \sin\theta \left[\eta'''(L_r)\right]^{2/3}} \,, \qquad \dots . (79)$$

This formula, derived by Ford and Wheeler (1959) is a special case of the famous result of Airy (1838) on light intensity near a caustic (he had the optical rainbow in mind).

We can now see very clearly just what the uniform approximation does : (79) shows that, very near θ_r, $\sigma_r(\theta)$ is of the order $\hbar^{-1/3}$. But (61) shows that, far from θ_r, $\sigma_r(\theta)$ is of order $\hbar^0$. Our general results, (75) - (77), interpolate smoothly between these regions of different analytic behaviour.

It is interesting to make a numerical comparison between the uniform approximation to $\sigma_r(\theta)$ and an exact calculation, based on summing the terms in the partial-wave series (47). Hundhausen and Pauly (1965) have performed such exact calculations for the Lennard-Jones potential used to describe intermolecular forces; this is

$$V(r) = \varepsilon\left\{\left(\frac{r_m}{r}\right)^{12} - 2\left(\frac{r_m}{r}\right)^6\right\},$$

where ε is the depth of the potential minimum, and r_m the radial distance at which it occurs (r_m is a measure of the size of the scatterer).

The case to be considered is defined by the parameter values

$$\frac{E}{\mathcal{E}} = 4.7$$

$$\frac{(2mE)^{1/2} r_m}{\hbar} = 346.$$

The ratio $E/\mathcal{E}$ defines the classical problem; the appropriate energy relationship is sketched in figure 19.

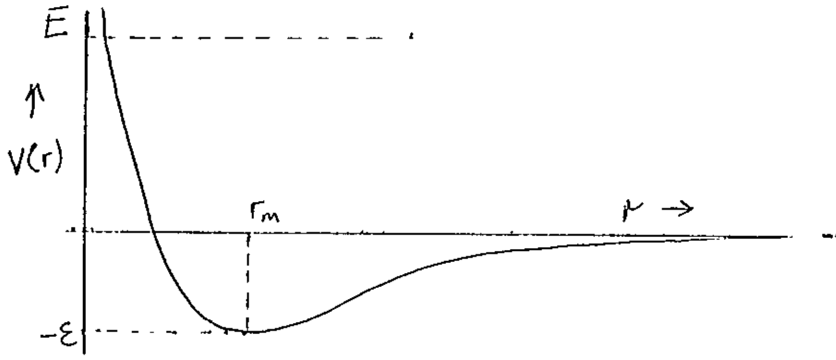

Figure 19. Energy relationships for scattering in Lennard-Jones potential.

The quantity $(2mE)^{1/2} r_m/\hbar$ is a measure of the wave-likeness of the problem, and in this case indicates that about 346 de Broglie wavelengths of the incident particle fit into the space occupied by the scatterer.

The rainbow cross section, calculated from our formula (76), is shown in figure 20, which also shows the classical approximation, the Airy approximation and the result of the exact calculation of Hundhausen and Pauly. The uniform approximation has not been used into the shadow because it only differs from the Airy approximation at angles where $\sigma_r(\theta)$ is negligible in comparison with its values in the lit region. The calculations of $\sigma_r(\theta)$ are presented in units of πr_m^2, the projected area of the scatterer. Because it was not possible to interpret the scale of the ordinates for the curves in the paper of Hundhausen and Pauly, these are drawn in figure 20 with the height of the maximum near $\theta = 12^\circ$ being made to agree with that calculated using (76); this is of course a somewhat arbitrary step.

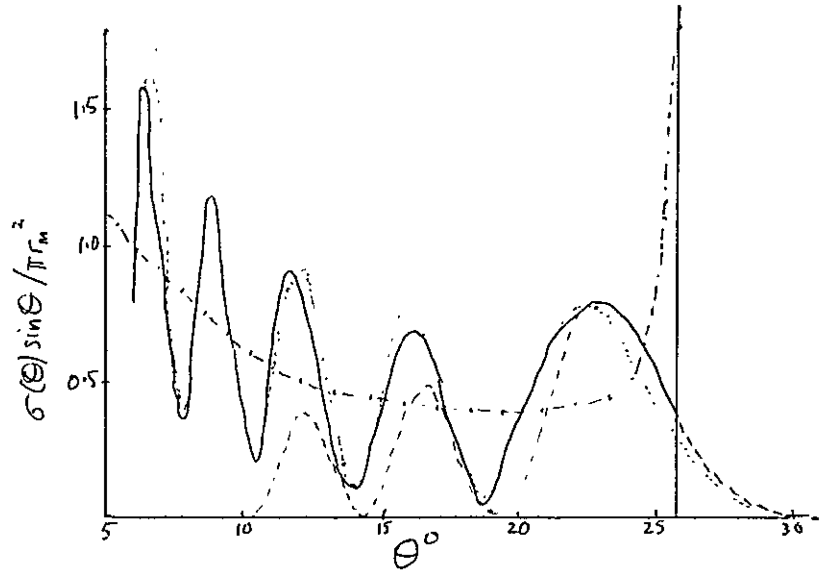

Figure 20. Comparison of different approximations for the rainbow cross section. Full curve, uniform approximation (equation (76) of text); dotted curve, exact calculation of Hundhausen and Pauly; broken curve, Airy approximation; chain curve, classical approximation.

It is clear that the uniform approximation mirrors the exact behaviour rather well. The worst discrepancies occur very close to the rainbow angle; these could well be errors of calculation, since our calculations of the classical and Airy approximations disagree in this angular region from those of Hundhausen and Pauly.

6. Glory Scattering

Let us consider what happens to the three contributing paths for the deflection function of figure 17, for the case of small angles of observation. The an ular momentum $L_1(\theta)$ of the outermost path then becomes ve y large, and the rays L_3 and L_2 approach one another, meeting at L_g when $\theta = 0$; all three terms of the stationary-phase result (61) diverge, and we must examine the reasons for this.

For all three rays the $1/\sin\theta$ factor causes a divergence; this factor originated when we replaced the uniform approximation (51) for $P_\ell(\cos\theta)$ by its asymptotic form. This is clearly wrong for small θ. But in the case of the path L_1 there occurs, in addition, the vanishing of the denominator $\frac{d\Theta(L)}{dL}$; The scattering cross-section then depends on the analytic form of the tail of the potential (just as the scattering length did for $\ell = 0$ in §3). All continuous potentials exhibit this dependence of the near-forward scattering on the rays with large angular momenta; This problem has been treated in the literature (Mason etal 1964, Keller and Levy 1963), for very small angles, but as far as I know nobody has derived approximations uniform in angle, which reduce to the final term of (61) when θ is fairly large.

We shall not consider this important but extremely difficult problem, but consider instead the scattering caused by the two paths L_3 and L_1. It is intuitively clear that any potential with a classical path which emerges in the forward direction for some finite L will have a characteristic small angle scattering pattern. This effect is a result of the three-dimensional nature of the scattering; away from the forward direction we get contributions from paths through θ and $-\theta$, but at $\theta = 0$ these degenerate into the same path (in the two-dimensional problem of scattering by a cylinder, the angles θ and $-\theta$ are observationally distinguishable and the divergence does not arise - the angular eigen functions are $e^{\pm im\theta}$ and not $P_\ell(\cos\theta)$, so there is no $\frac{1}{\sin\theta}$ factor). An analogous situation occurs with rays emerging in the backward direction. This phenomenon, which we call Glory scattering, arises whenever the deflection function Θ (L) passes smoothly through a multiple of π . The name is taken from a partially analogous optical effect involving the strong back - scattering of light from water droplets; however, in this case the system of rays does not quite reach round to $\theta = \pi$, and the analysis is complicated by the need to include rays which creep round the sphere to the backward direction (see Van de Hulst 1957, Nussenzweig 1966).

For the deflection function of fig. 17, we have a forward glory at $\Theta = 0$. Analytically therefore, we have to evaluate just the m = 0 term of the series (52), namely

$$f(\theta) = \frac{-i}{\hbar}\left(\frac{\theta}{2mE\sin\theta}\right)^{1/2}\int_0^\infty dL\, L\, J_0\left(\frac{L\theta}{\hbar}\right)\left[e^{\frac{2i\tilde{\eta}(L)}{\hbar}} - 1\right], \tag{80}$$

since it is this term which, when the Jo is expanded asymptotically, yields the two integrals $I_0^{\pm}$.

It is easy enough to get a transitional approximation, since when θ is very small $(O(\frac{\hbar}{L_{class}}))$, the Bessel function oscillates very slowly along the L-axis; there are then two separate contributions, from the stationary points of the exponential factor at L = Lg and $L \rightarrow \infty$. Thus we write:-

$$f(\theta) = f_g(\theta) + f_{tail}(\theta) \tag{81}$$

and forget about f_{tail}. The glory part, for these very small angles, can be obtained from the simple stationary-phase method as

$$f_g(\theta) \simeq -i\left(\frac{\pi\theta}{mE\hbar\sin\theta\,|\Theta'(L_g)|}\right)^{1/2} L_g\, J_0\left(\frac{L_g\theta}{\hbar}\right) e^{\frac{2i\tilde{\eta}(L_g)}{\hbar} - \frac{i\pi}{4}}, \tag{82}$$

or

$$\sigma_g(\theta) \simeq \frac{\pi\theta L_g^2\, J_0^2\left(\frac{L_g\theta}{\hbar}\right)}{mE\sin\theta\,|\Theta'(L_g)|\,\hbar} \tag{83}$$

a result first obtained by Ford and Wheeler (1959), showing that the glory cross-section changes from being $O(\hbar^0)$ for $\Theta \gg 0$ to $O(\hbar^{-1})$ at $\theta = 0$.

It is rather more difficult to get a uniform approximation in this case than for the rainbow, but it is also more important to do so, since we have shown $\sigma(\theta)$ to vary over a wider range of values near a glory than near a rainbow, and an inaccurate description in the range between the transitional and semiclassical approximations will show up more strongly. We shall work out the rather more general integral:-

$$I \equiv \int_0^\infty f(L)\, e^{\frac{2i\tilde{\eta}(L)}{\hbar}}\, J_0\!\left(\frac{L\Theta}{\hbar}\right) dL . \tag{84}$$

We have now omitted the -1 term which occurs in (80); this term is necessary to make the integral converge for large L but only contributes explicitly to f_{tail}. We immediately convert the Jo into exponential form by using a standard integral representation, which gives us the double integral

$$I = \frac{1}{\pi} \int_0^\pi d\phi \int_0^\infty dL\, f(L)\, e^{\frac{i}{\hbar}\left[2\tilde{\eta}(L) + L\Theta\cos\phi\right]} . \tag{85}$$

Let us look first at the integral over L. The exponent has one stationary point, $L = L_0(\Theta,\phi)$, satisfying

$$2\frac{d\tilde{\eta}}{dL} = \Theta'(L) = -\Theta\cos\phi .$$

As ϕ varies from 0 to π , $L_0(\Theta,\phi)$ varies from $L_2(\Theta)$ to $L_3(\Theta)$ (see fig 17); since $\Theta'(L)$ never vanishes in this range we may use the ordinary method of stationary phase to evaluate the L integral, to get the result, uniformly valid in ϕ ,

$$I = \sqrt{\frac{2\hbar}{\pi}}\, e^{-\frac{i\pi}{4}} \int_0^\pi d\phi\, \frac{f\left(L_0(\Theta,\phi)\right)}{\sqrt{\left|\Theta'\left(L_0(\Theta,\phi)\right)\right|}}\, e^{\frac{i}{\hbar}\left[2\tilde{\eta}\left(L_0(\Theta,\phi)\right) + L_0(\Theta,\phi)\Theta\cos\phi\right]} \tag{86}$$

To deal with the ϕ - integral we notice that those parts of the integrand involving Lo vary only slowly over the range of ϕ ; most of the functional dependence comes from the cos ϕ term. There are two stationary points, at the limits of integration $\phi = 0$ and $\phi = \pi$ (because these values satisfy

$$\left(2\frac{d\tilde{\eta}(L_0(\Theta,\phi))}{dL} + \Theta\cos\phi\right)\frac{dL_0(\Theta,\phi)}{d\phi} - L_0(\Theta,\phi)\Theta\sin\phi = 0$$

).

We retain this behaviour if we map ϕ onto a new integration variable ψ by the substitution

$$2\tilde{\eta}\left(L_0(\Theta,\phi)\right) + L_0(\Theta,\phi)\Theta\cos\phi \equiv a(\Theta) + b(\Theta)\cos\psi . \tag{87}$$

As in all our earlier derivations of uniform approximations we demand that the mapping is one-to-one; in this case we must have the correspondences:-

$$\phi = 0 \longleftrightarrow \psi = 0$$

$$\phi = \pi \longleftrightarrow \psi = \pi,$$

which lead to

$$\left.\begin{aligned} a(\theta) &= \frac{S_2(\theta) + S_3(\theta)}{2} \equiv \overline{S(\theta)} \\ b(\theta) &= \frac{S_2(\theta) - S_3(\theta)}{2} \equiv \frac{\Delta S(\theta)}{2} \end{aligned}\right\} \qquad (88)$$

Thus, just as in the rainbow case, what is involved are the mean and difference of the actions along the two contributing classical paths. Using (88) and (87), our integral (86) becomes

$$I = \frac{\sqrt{2\pi\hbar}\, e^{-\frac{i\pi}{4} + \frac{i\overline{S}(\theta)}{\hbar}}}{\pi} \int_0^\infty d\psi \frac{f(L_0(\theta,\phi(\psi)))}{\sqrt{|\Theta'(L_0(\theta,\phi(\psi)))|}} \frac{d\phi(\psi)}{d\psi} e^{i\frac{\Delta S(\theta)}{2\hbar}\cos\psi} \qquad (89)$$

To evaluate the integral, we need to approximate the slowly-varying function

$$g(\psi) = \frac{f(L_0(\theta,\phi(\psi)))}{\sqrt{|\Theta'(L_0(\theta\phi(\psi)))|}} \frac{d\phi}{d\psi}(\psi) \qquad (90)$$

which multiplies the exponential. Now, when θ is large, ΔS is large, the integrand oscillates violently and the only contributions come from the stationary points, while when θ is small $g(\psi)$ is almost a constant (since Lo is always near to L_F). Thus if we write:-

$$g(\psi) = p + q\cos\psi + \sin\psi\, h(\psi)$$

then since the third term is zero at the stationary points we do not expect it to contribute much to the integral, so we neglect it. The resulting expressions are easy to calculate, and we have

$$I = \sqrt{2\pi\hbar}\, e^{-\frac{i\pi}{4} + \frac{i\overline{S}(\theta)}{\hbar}} \left[p J_0\left(\frac{\Delta S(\theta)}{2\hbar}\right) - iq J_0'\left(\frac{\Delta S(\theta)}{2\hbar}\right)\right]. \qquad (91)$$

For P and Q we have, from (91) and (90),

$$\left.\begin{aligned} p &= \frac{1}{2}\left[\frac{f(L_2(\Theta))}{\sqrt{|\Theta'(L_2(\Theta))|}}\frac{d\phi}{d\psi}(0) + \frac{f(L_3(\Theta))}{\sqrt{|\Theta'(L_3(\Theta))|}}\frac{d\phi}{d\psi}(\pi)\right] \\ q &= \frac{1}{2}\left[\frac{f(L_2(\Theta))}{\sqrt{|\Theta'(L_2(\Theta))|}}\frac{d\phi}{d\psi}(0) - \frac{f(L_3(\Theta))}{\sqrt{|\Theta'(L_3(\Theta))|}}\frac{d\phi}{d\psi}(\pi)\right] \end{aligned}\right\} \qquad (93)$$

To evaluate the derivatives $\frac{d\phi}{d\psi}$ we differentiate the mapping relation (87) twice; the first time giving

$$\left(2\frac{d\tilde{\eta}(L_0)}{dL} + \Theta\cos\phi\right)\frac{dL_0}{d\phi}\frac{d\phi}{d\psi} - L_0\Theta\sin\phi\frac{d\phi}{d\psi} = -b\sin\psi .$$

The first term is always zero because of the definition of $L_0(\Theta,\phi)$, while the next two terms are both zero at $\psi = 0$ or π. A second differentiation gives

$$-\Theta\sin\phi\frac{dL}{d\phi}\left(\frac{d\phi}{d\psi}\right)^2 - L_0\Theta\cos\phi\left(\frac{d\phi}{d\psi}\right)^2 - L_0\Theta\sin\phi\frac{d^2\phi}{d\psi^2} = -b\cos\psi,$$

or

$$\frac{d\phi}{d\psi}(0) = \sqrt{\frac{+b(\Theta)}{\Theta L_2(\Theta)}} \quad ; \quad \frac{d\phi}{d\psi}(\pi) = \sqrt{\frac{b(\Theta)}{\Theta L_3(\Theta)}} .$$

If we put these relations into (93), (93) into (92) and we use (88), we finally get our uniform approximation to (84):

$$\boxed{\begin{aligned} I = \sqrt{\frac{\pi\hbar\Delta S(\Theta)}{2\Theta}}\, e^{-\frac{i\pi}{4} + i\frac{\bar{S}(\Theta)}{\hbar}} \Bigg\{ &\left(\sqrt{\frac{1}{L_2|\Theta_2'|}}\, f(L_2) + \sqrt{\frac{1}{L_2|\Theta_3'|}}\, f(L_3)\right) J_0\left(\frac{\Delta S(\Theta)}{2\hbar}\right) - \\ &- i\left(\sqrt{\frac{1}{L_2|\Theta_2'|}}\, f(L_2) - \sqrt{\frac{1}{L_3|\Theta_3'|}}\, f(L_3)\right) J_0'\left(\frac{\Delta S(\Theta)}{2\hbar}\right) \Bigg\} \end{aligned}} \qquad (94)$$

The reason why we have evaluated this more general integral with the factor f(L) in the integrand is that we can check the result against an exactly known integral, namely,

$$\begin{aligned} I &\equiv \int_0^\infty \frac{dL}{L}\, e^{-\frac{i}{\hbar}\left(L\gamma + \frac{1}{L\delta}\right)} J_0(L\Theta/\hbar) \\ &= -i\pi H_0^{(2)}\left[\frac{\left(\sqrt{\gamma+\Theta} + \sqrt{\gamma-\Theta}\right)}{\hbar\sqrt{\delta}}\right] J_0\left[\frac{\left(\sqrt{\gamma+\Theta} - \sqrt{\gamma-\Theta}\right)}{\hbar\sqrt{\delta}}\right] \end{aligned} \qquad (95)$$

(Ryzhik and Gradshteyn 1965)

This corresponds to taking

$$f(L) = L^{-1} \;;\quad 2\tilde{\eta}(L) = -L\gamma - \frac{1}{L\delta}\,. \tag{96}$$

This is an ideal model phase shift for our purposes, since it has just a single stationary point on the range of integration, at $L = L_g = \frac{1}{\sqrt{\gamma\delta}}$; it does not go to zero at $L = \infty$ like a real phase shift, so we have no trouble with f tail (θ).

We have $\Theta(L) = -\gamma + \frac{1}{\delta L^2}$

so that $\frac{1}{\delta L_2^2} = \gamma - \theta \quad , \frac{1}{\delta L_3^2} = \gamma + \theta$

and $\qquad L_2 = \frac{1}{\sqrt{\delta(\gamma-\theta)}} \quad , L_3 = \frac{1}{\sqrt{\delta(\gamma+\theta)}}\,.$

For the action,

$$S_2 = -L_2\gamma - \frac{1}{L_2\delta} + L_2\theta = -2\sqrt{\frac{\gamma-\theta}{\delta}}\;;$$

$$S_3 = -L_3\gamma - \frac{1}{L_3\delta} - L_3\theta = -2\sqrt{\frac{\gamma+\theta}{\delta}}\;,$$

So that

$$\bar{S}(\theta) = -\left(\frac{\sqrt{\gamma-\theta}+\sqrt{\gamma+\theta}}{\sqrt{\delta}}\right)$$

$$\Delta S(\theta) = \frac{2}{\sqrt{\delta}}\left(\sqrt{\gamma+\theta} - \sqrt{\gamma-\theta}\right).$$

Finally we need

$$\Theta'(L_2) = -\frac{2}{\delta L_2^3} = -2\sqrt{\delta}\,(\gamma-\theta)^{3/2}$$

$$\Theta'(L_3) = -2\sqrt{\delta}\,(\gamma+\theta)^{3/2}.$$

When we substitute all these results into our formula (94), the term in J_0' happens to be zero (this is presumably why it is the integral with $f(L) = \frac{1}{L}$ that is tabulated rather than the general case $f(L) = L^n$ which can be derived from (95) by differentiation with respect to γ), and we are left with the simple result,

$$I \approx \sqrt{\pi\hbar}\;\delta^{1/4}\sqrt{\frac{(\sqrt{\gamma+\theta}-\sqrt{\gamma-\theta})}{\theta}}\;e^{-\frac{i\pi}{4}-\frac{i(\sqrt{\gamma-\theta}+\sqrt{\gamma+\theta})}{\hbar\sqrt{\delta}}}\;J_0\left(\frac{(\sqrt{\gamma+\theta}-\sqrt{\gamma-\theta})}{\hbar\sqrt{\delta}}\right) \tag{97}$$

to be compared with the exact result (95). Now we expect our approximation to be valid uniformly in θ when $\hbar$ is small and γ and δ are of zero order in $\hbar$; thus the Hankel function $H_0^{(2)}$ in (95) has a large argument and we may use the asymptotic approximation for it. When we do this, the result is the formula (97); we cannot approximate Jo because its argument is small when $\theta = 0(\hbar)$. Our uniform approximation therefore does everything expected of it for this special case.

For the scattering amplitude in which we are interested, f (L) = L, and our uniform approximation for (80) is

$$\boxed{f_g(\theta) = \frac{1}{2}\sqrt{\frac{\pi\Delta S(\theta)}{2\hbar m E\sin\theta}}\; e^{-\frac{3\pi i}{4} + i\frac{\bar{S}(\theta)}{\hbar}}\left\{\left(\sqrt{\frac{L_2}{|\Theta_2'|}} + \sqrt{\frac{L_3}{|\Theta_3'|}}\right) J_0\left(\frac{\Delta S(\theta)}{2\hbar}\right) - i\left(\sqrt{\frac{L_2}{|\Theta_2'|}} - \sqrt{\frac{L_3}{|\Theta_3'|}}\right) J_0'\left(\frac{\Delta S(\theta)}{2\hbar}\right)\right\}.} \qquad (98)$$

This is very similar in form to the rainbow integral (75); the scattering involves quantities occuring in the purely classical problem - actions, densitites of paths etc., but these are involved in Bessel functions instead of exponentials. Our general formula should give the semiclassical and transition approximations in the appropriate cases; away from the forward direction, the difference in action between the two contributing paths is many units of $\hbar$, and we can replace the Bessel functions by their asymptotic forms. This leads exactly to the semiclassical result (61) (without the term from the "tail" path L_1). Very close to $\theta = 0$ we expand the action about the glory ray

$$2\tilde{\eta}(L) - L\Theta = 2\tilde{\eta}(L_g) - L_g\Theta - (L - L_g)\Theta - \frac{|\Theta'(L_g)|}{2}(L - L_g)^2 + \cdots$$

which on differentiation gives the contributing angular momenta as

$$L_{\substack{2\\3}} = L_g - \frac{\Theta_{\substack{2\\3}}}{|\Theta_g'|} = L_g \pm \frac{\theta}{|\Theta'(L_g)|},$$

and the corresponding actions as

$$S_{\substack{2\\3}}(\theta) = 2\tilde{\eta}(L_g) + \theta^2/2|\Theta_g'| \pm L_g\theta$$

$$\simeq 2\tilde{\eta}(L_g) \pm L_g\theta.$$

When we substitute these results into (9.) we can neglect the term in J_0' since it is $O(\theta^2)$ relative that involving Jo. We than get precisely the transitional approximation (82).

This concludes our treatment of semiclassical scattering. There still remains work to be done on the uniform approximation of the contribution from the potential tails in the neighbourhood of the forward direction; also, we have said nothing about the scattering from orbiting, which occurs when there are metastable states localised near $r = 0$ (see Ford and Wheeler 1959)

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7. An integral from Fermiology:- the de Haas van Alphen effect for an hourglass shaped Fermi surface.

A full treatment of the motion of the Bloch electrons in a metal under the action of a magnetic field H is very complicated (see Chambers 1966); for many purposes it is sufficient to replace the effect of the atomic potentials by an effective hamiltonian operator $H(\underline{P})$ which is constant in space and gives the electron energy as a function of its momentum $\underline{P}$ (Pippard, 1965). In metal physics we usually specify the motion by the wave vector $\underline{k} = \frac{\underline{P} - e\underline{A}/c}{\hbar}$ When a magnetic field is applied the $\underline{k}$-value of the particle moves round an orbit on a constant-energy surface; the plane of the orbit is perpendicular to $\underline{H}$; associated with this $\underline{k}$-space orbit is a real space orbit, which has a magnetic moment. The total magnetic moment of the whole assembly of conduction electrons is composed of two parts. First, steady Landau diamagnetism : this is a subtle effect which is zero in the classical limit, but which appears in the first semiclassical correction term. We shall be concerned with the second part of the magnetic moment, which is an oscillating function of the field $\underline{H}$; this is the de-Haas van Alphen effect. It arises from levels squeezing past the fermi energy, and its value is given by

$$M_{osc} = \frac{kT}{2\pi^2 H \sinh\left(\frac{2\pi^2 kTm_f}{e\hbar H}\right)} \underline{I}, \tag{99}$$

where

$$\underline{I} = \int dk_z \, A(k_z) \sin \frac{A(k_z)\hbar}{eH}, \tag{100}$$

(Pippard 1968, Ziman 1964). In these formulae, T is the temperature, m_f the cyclotron effective mass on the Fermi surface, and A (k_z) is the area of that orbit in k-space at the Fermi energy which has wave vector component k_z along the magnetic field direction (see figure 21); this orbit is thus a section of the Fermi surface. It is the integral (100) that will concern is here. Similar integrals arise in the theory of transport properties in a thin film (Chambers 1968).

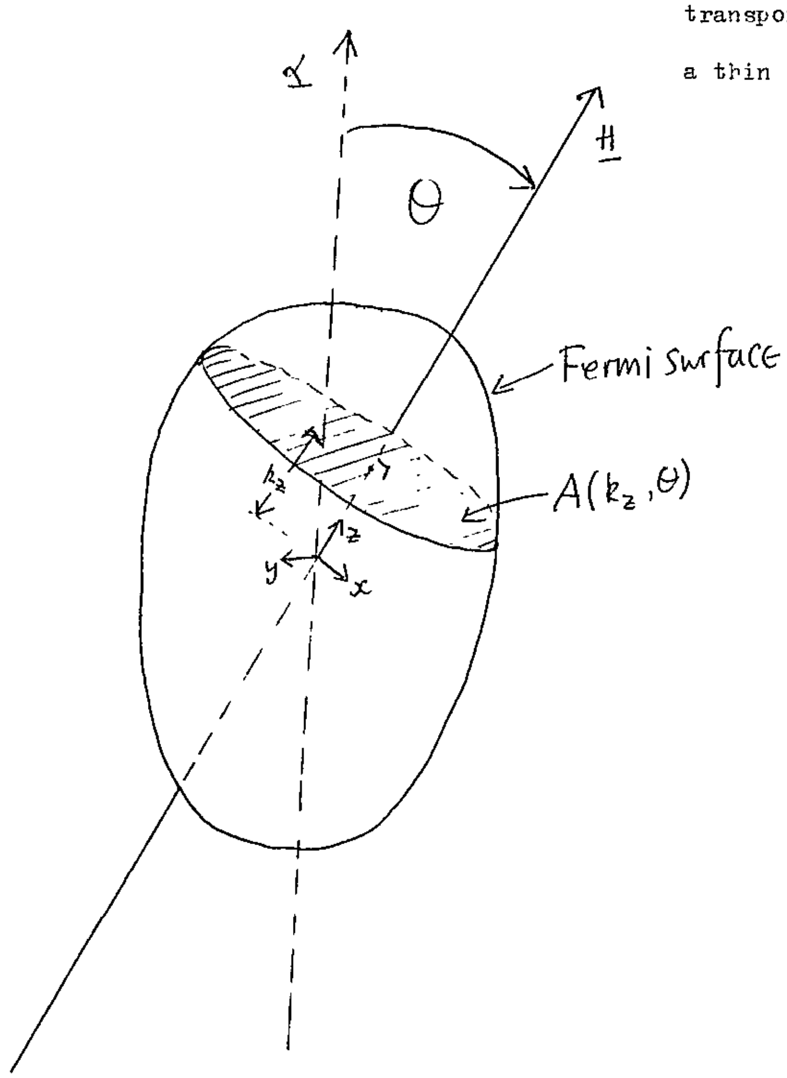

Figure 21. Orbit on Fermi surface in magnetic field.

To see that this is a semiclassical integral we realise that classical orbits have momenta of order $\hbar k$, so the classical area in momentum units corresponding to A is $\frac{A}{\hbar^2}$ which indicates that the sine in (100) has a phase of the type $\frac{\text{classical quantity}}{\hbar}$. It is convenient for this example to think of the small semiclassical parameter as the magnetic field H. Thus asymptotic methods are appropriate for evaluating it. This means that the extremal orbits where k_z has a value, K, such that A(K) is an extremum, will give the dominant contributions to the integral. (For a closed Fermi surface there will also be elliptic limiting-point oscillations, corresponding to the finite limits of the integral where the orbit has degenerated into a point of zero area. These give a lower-order contribution than the extremal orbits, but can still be observed (Chambers 1968 gives a full treatment)§.

If we restrict ourselves to Fermi surfaces which are rotationally symmetric about some axis $\underline{\alpha}$, then only the angle θ, made by $\underline{H}$ with $\underline{\alpha}$, (figure 21) is needed to describe the dependence of the pattern on the field direction. (We shall indicate this by denoting orbit areas by $A(k_z, \theta)$). The simplest type of Fermi surface is closed and convex everywhere. Then there is only one extremal orbit (a maximum or belly orbit), whatever the value of θ, which gives a simple semiclassical contribution to the integral (100) unless the curve generating the surface is nearly flat over any substantial portion of its length; however, this case (which occurs when there are long cigar-shaped bits of surface) is easily dealt with by the theory of stationary points of higher order.

We are not here concerned with enumerating all the types of orbit that can occur for various angles θ on an arbitrary Fermi surface (for this, see Pippard 1965); rather, we are discussing the precise analytical description of the simplest cases, and from this point of view the next most complicated case is the hourglass-shaped surface of figure (22).

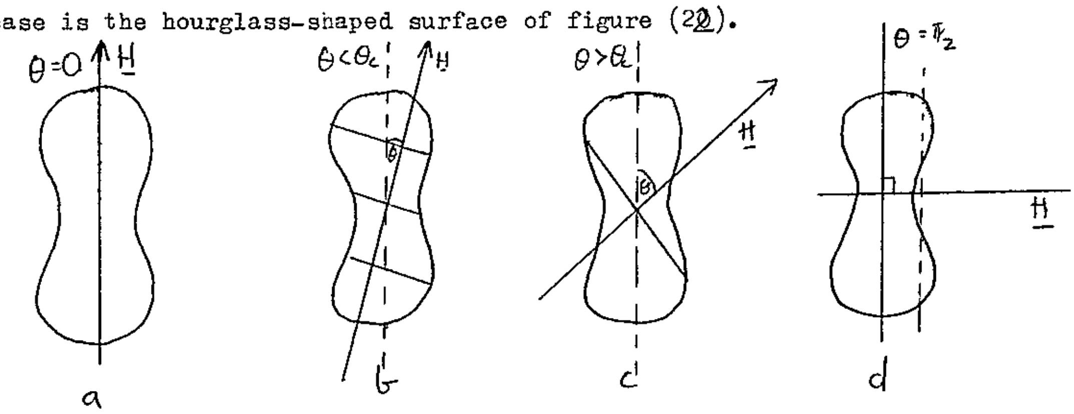

Fig 22: Extremal Orbits on hourglass-shaped Fermi surface.

The topology of the extremal orbits changes with Θ: when $\underline{H}$ points nearly along the axis of symmetry of the fermi surface, there are three extremal orbits, two maxima round the (cylindrically symmetric!) bosom and hips at $k_z = \pm k(\Theta)$, and a minimum waist orbit at $k_z = 0$ (a and b). When Θ exceeds a critical angle Θ_c, however, there is only one extremal orbit, a maximum at $\Theta = 0$ (c and d). This still holds even when, for Θ greater than a second critical angle, the ends of the range of integration contain contributions from two orbits as in the dotted line on Fig. 20d.

The semiclassical approximation to the integral (100), valid when $\Theta \ll \Theta_c$ is

$$I \approx \sqrt{\frac{2\pi eH}{\hbar}}\left[\frac{2A(k(\Theta),\Theta)}{\sqrt{-\frac{d^2A(k(\Theta),\Theta)}{dk_z^2}}}\sin\left(\frac{\hbar}{eH}A(k(\Theta),\Theta)-\pi/4\right)+\right.$$
$$\left.+\frac{A(0,\Theta)}{\sqrt{\frac{d^2A(0,\Theta)}{dk_z^2}}}\sin\left(\frac{\hbar}{eH}A(0,\Theta)+\pi/4\right)\right], \qquad (101)$$

showing the two oscillations from the two kinds of orbit. When $\Theta \gg \Theta_c$ the analogous result is

$$I \approx \sqrt{\frac{2\pi eH}{\hbar\left(-\frac{d^2A(0,\Theta)}{dk_z^2}\right)}}\; A(0,\Theta)\sin\left(\frac{\hbar}{eH}A(0,\Theta)-\frac{\pi}{4}\right). \qquad (102)$$

Now, if we want a uniformly approximate description, we have to map the exponent in (100) onto a function of a new variable x, which has three real stationary points for a 0, maxima at $x = \pm\sqrt{a}$ and a minimum at $x = 0$, and a single real stationary point at a 0, a maximum at $x = 0$. Such a mapping is the quartic expression:-

$$\frac{\hbar A(k_z,\Theta)}{eH} = b(\Theta) - \left(x^2 - a(\Theta)\right)^2, \qquad (103)$$

For the mapping to be 1 - 1 we must make the stationary points correspond, or

$$k_z = 0 \longleftrightarrow x = 0$$
$$k_z = \pm k(\theta) \longleftrightarrow x = \pm\sqrt{a} \tag{104}$$

which leads to

$$\left.\begin{aligned} b(\theta) &= \frac{\hbar}{eH} A(k(\theta),\theta) \\ a(\theta) &= \left(\frac{\hbar}{eH}\left(A(k(\theta),\theta) - A(0,\theta)\right)\right)^{1/2} \end{aligned}\right\}, \tag{105}$$

In terms of the new variable, the integral (100) is

$$I = \mathcal{J}_m e^{ib(\theta)} \int_{-\infty}^{\infty} dx \frac{dk_z}{dx} A(k_z,\theta)\, e^{-i(x^2-a(\theta))^2}, \tag{106}$$

where we have written the limits as $\pm\infty$ in accordance with our decision to ignore the limiting-point oscillations.

To be able to do the integral we need to expand the $A\frac{dk_z}{dx}$ factor about the stationary points. Now $A(k_z,\theta)$ is even, so that $k_z(x)$ is oddd and $\frac{dk_z}{dx}$ is even too; a suitable expansion is thus

$$\frac{dk_z}{dx} A(k_z(x),\theta) = p + qx^2 + x(x^2-a)\, g(x), \tag{107}$$

and according to the argument we have used several times before, we may neglect the last term. There are several forms in which we may evaluate the integral (106), but for the most convenient we refer to Felsen (1964) p. 10.) The result is

$$I = \frac{\mathcal{J}_m\sqrt{\pi}}{2^{1/4}} e^{i\left[b(\theta) - \frac{a^2(\theta)}{2}\right]} \left\{ p e^{-\frac{i\pi}{8}} D_{-1/2}\left(a(\theta)\sqrt{2}\, e^{-\frac{3\pi i}{4}}\right) + \frac{q\, e^{-\frac{3\pi i}{8}}}{2^{3/2}} D_{-3/2}\left(a(\theta)\sqrt{2}\, e^{-\frac{3\pi i}{4}}\right)\right\}, \tag{108}$$

Where the $D_\nu(z)$ are parabolic cylinder functions ,

Now, from (107) we easily get

$$\left.\begin{aligned} p &= \frac{dk_z(0)}{dx} A(0,\theta), \\ q &= \frac{1}{a}\left[\frac{dk_z(k(\theta))}{dx} A(k(\theta),\theta) - \frac{dk_z(0)}{dx} A(0,\theta)\right] \end{aligned}\right\}, \tag{109}$$

To find the derivatives $\frac{dk_z}{dx}$ at the stationary points we follow our familiar procedure of doubly differentiating the mapping relation (107) with respect to x. This gives

$$\frac{\hbar}{eH}\frac{dA}{dk_z}\frac{dk_z}{dx} = -4x(x^2-a),$$

and

$$\frac{\hbar}{eH}\left[\frac{d^2A}{dk_z^2}\left(\frac{dk_z}{dx}\right)^2 + \frac{dA}{dk_z}\frac{d^2k_z}{dx^2}\right] = 4a - 12x^2, \tag{110}$$

so that

$$\frac{dk_z(0)}{dx} = \sqrt{\frac{4a(\theta)eH}{\hbar\frac{d^2A}{dk_z^2}(0,\theta)}}\;;\;\frac{dk_z(k(\theta))}{dx} = \sqrt{\frac{-8a(\theta)eH}{\hbar\frac{d^2A}{dk_z^2}(k(\theta),\theta)}}\,. \tag{111}$$

If we insert this into (109) and (110), we finally get, as our uniform approximation to the integral (100):

$$\boxed{\begin{aligned} I = {} & J_m 2^{3/4}\sqrt{\pi}\left(\frac{eH}{\hbar}\Delta A(\theta)\right)^{1/4} e^{i\frac{\bar{A}(\theta)\hbar}{He}}\left\{ e^{-\frac{i\pi}{8}}\frac{A(0,\theta)}{\sqrt{\frac{d^2A}{dk_z^2}(0,\theta)}}\, D_{-\frac{1}{2}}\left(e^{-\frac{3\pi i}{4}}\sqrt{\frac{2\hbar}{eH}\Delta A(\theta)}\right) + \right. \\ & \left. + \frac{e^{-\frac{3\pi i}{8}}}{2\left(\frac{2\hbar}{eH}\Delta A(\theta)\right)^{1/2}}\left[\sqrt{\frac{2}{-\frac{d^2A}{dk_z^2}(k(\theta),\theta)}}\,A(k(\theta),\theta) - \frac{A(0,\theta)}{\sqrt{\frac{d^2A}{dk_z^2}(0,\theta)}}\right] D_{-\frac{3}{2}}\left(e^{-\frac{3\pi i}{4}}\sqrt{\frac{2\hbar}{eH}\Delta A(\theta)}\right)\right\}, \end{aligned}} \tag{112}$$

where $\bar{A}(\theta)$ and $\Delta A(\theta)$ are the mean and difference respectively of the two extremal areas involved.

As in our earlier examples, we shall examine this result in the three regions of interest. The simplest is $\theta \ll \theta_c$, when there are three real extremal orbits, and we require the asymptotic approximations to the $D_\nu(z)$ where the phase of z is $\frac{3\pi i}{4}$. These are

$$D_{-\frac{1}{2}}(z) \simeq \frac{e^{-z^2/4}}{\sqrt{z}} - i\sqrt{2}\,\frac{e^{+z^2/4}}{\sqrt{z}}\;;\; D_{-\frac{3}{2}}(z) \simeq i\,2\sqrt{2z}\;e^{z^2/4}. \tag{113}$$

If we use these in (112) we regain precisely the semiclassical result (101).

When $\theta \gg \theta_c$ the bust and hip orbits at $k_z = \pm k(\theta)$ now have complex k_z, but $A\ (k(\theta))$ is still real because $A\ (k_z)$ is an even function; we still have $A\ (k(\theta)) > A(0)$, so that $\Delta A > 0$ and we can still make $a\ (\theta)$ in (105) real (as we have to for the mapping (103) to be real), but now it is argument 2π. The argument of the $D_v(z)$ is now $\sqrt{\frac{2\hbar}{eH}|\Delta A|}\ e^{i\pi/4}$, and the appropriate asymptotic forms are

$$D_{-\frac{1}{2}}(z) \sim \frac{e^{-z^2/4}}{z^{1/2}} \quad ; \quad D_{-\frac{3}{2}}(z) \sim \frac{e^{-z^2/4}}{z^{3/2}} \ . \tag{114}$$

The term in $D_{-\frac{3}{2}}$ is of higher order in H than that in $D_{-\frac{1}{2}}$ so we can neglect it. When we apply this asymptotic form we get exactly the semiclassical result (102).

To derive the transitional approximation, we must expand the area near to $k_z = 0$ and $\theta = \theta_c$. The lowest order suitable expansion is

$$\left.\begin{aligned} A(k_z,\theta) &= \mathcal{A} + \frac{B(\theta_c-\theta)k_z^2}{2} - \frac{C}{4!}k_z^4 \\ \text{Where} \quad \mathcal{A} &= A(0,\theta_c)\ , \quad B = -\frac{\partial^3 A}{\partial k_z^2 \partial\theta}(0,\theta_c)\ , \\ C &= \frac{\partial^4 A}{\partial k_z^4}(0,\theta_c) \end{aligned}\right\} . \tag{115}$$

This gives

$$k(\theta) = \sqrt{\frac{3B}{C}(\theta_c-\theta)}$$

and

$$\Delta A(\theta) = \frac{9}{8}\frac{B^2}{C}(\theta_c-\theta)^2 .$$

In (112), we can neglect the term in $D_{-\frac{3}{2}}$ since this is of higher order in H than that in $D_{-\frac{1}{2}}$. The final result for the transitional approximation is

$$I = J_m\sqrt{\pi}\left(\frac{9eH}{\hbar C}\right)^{1/4}\mathcal{A}\, e^{-\frac{i\pi}{8}}\, D_{-\frac{1}{2}}\left[\frac{3B}{2}e^{-\frac{3\pi i}{4}}\sqrt{\frac{\hbar}{eHC}}\ (\theta_c-\theta)\right] . \tag{116}$$

If we compare this with (101) and (102) we see that near $\theta = \theta_c$ the de Haas Van Alphen effect is a factor $H^{-1/4}$ more intense than it is when θ is not near θ_c. A rough sketch of this transitional approximation is shown in Fig 23.

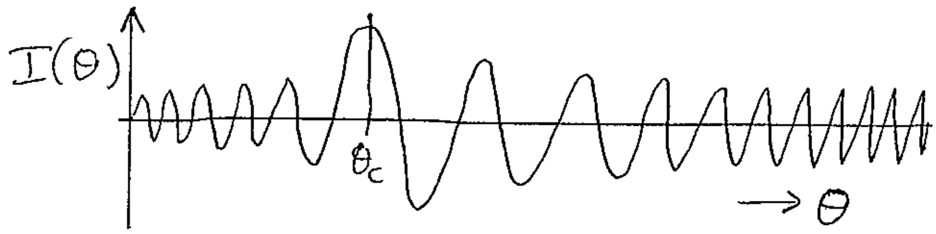

Fig. 23 De Haas Van Alphen effect near critical angle

The analytical relationship between the shape of the Fermi surface and the form of the area $A(k_z\theta)$ is rather complicated. To examine this matter we specify the surface originally by polar co-ordinates (r_0, θ_0, ϕ_0), whose z - axis is the axis of symmetry $\underline{\alpha}$. Bearing in mind the fact that we are treating rotationally symmetric surfaces whose top and bottom halves are the same, we can define the surface by the equation

$$r_0 = r_0(\theta_0) = \sum_{\ell=0}^{\infty} a_{2\ell} P_{2\ell}(\cos\theta_0) \tag{117}$$

and we must have at least a_0 and a_4 non zero in order to get the hourglass type of surface we are considering (see Fig. 24).

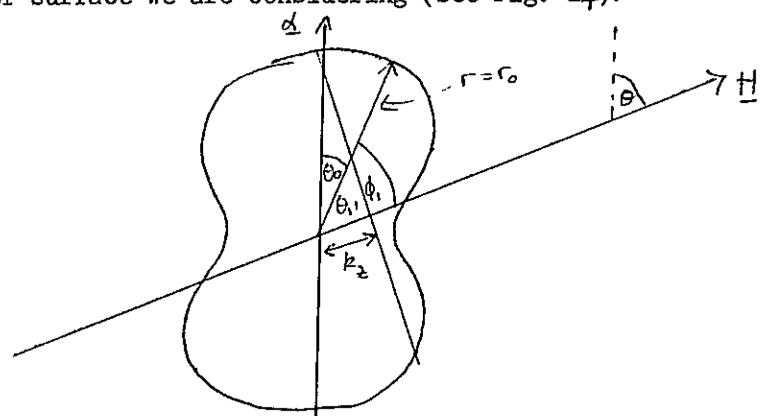

Fig 24. Co-ordinates used to evaluate areas

It is a straightforward application of the addition theorem of spherical harmonics to re-express the equation of the surface in polars (r, θ_1, ϕ_1) measured relative to $\underline{H}$. This gives

$$r = r(\theta_1, \phi_1) = \sum_{\ell=0}^{\infty} \frac{4\pi}{4\ell+1} a_{2\ell} \sum_{m=-2\ell}^{+2\ell} Y^*_{2\ell,m}(\theta,0)\, Y_{2\ell,m}(\theta_1,\phi_1) \; . \tag{118}$$

The boundary of the area $A(k_z\,\theta)$ is the intersection of this surface with the plane normal to H, given by

$$r \cos\theta_1 = k_z \tag{119}$$

This boundary curve is thus given by

$$r\ (\theta_1,\phi_1)\ \cos\ \theta_1 = k_z$$

or

$$\theta_1 = \theta_1\ (\phi_1, k_z, \theta) \qquad (120)$$

The area bounded by this curve is thus given by

$$A\left(k_z,\theta\right) = \frac{1}{2}\oint d\phi_1\ r^2 \sin\theta_1,$$

or

$$A(k_z,\theta) = \frac{1}{2}k_z^2\oint d\phi_1\ \frac{\tan\theta_1(\phi_1,k_z,\theta)}{\cos\theta_1(\phi_1,k_z,\theta)} \qquad (121)$$

This formula is difficult to evaluate in terms of the co-efficients $a_{2\ell}$ specifying the shape of the surface.

8. Waves in timevarying media: a frequency-modulator for lasers.

When considering monochromatic light, we tend to think of the frequency as the fundamental quantity; the wavelength, as we know, depends on the refractive index of the substance through which the light happens to be passing. But if we pass light through a medium whose refractive index varies with time, (a gas of variable density for instance), then it will, in theory, emerge with a changed frequency. This possibility (which must surely have occurred to many scientists over the last century) has recently been suggested by Duguay et al (1966) (see Teller 1967) as a means of modulating laser beams.

It is fitting for two reasons to end this report with the theory of these light waves in time-varying media. First, under almost all conceivable experimental conditions the asymptotic theory is almost exact without requiring any significant correction. Second, there are in this problem no critical points - caustics, turning points, and the like - such as have been responsible for the complexity of the formulae in the examples we have treated so far; this means that we can get a uniform approximation (valid for all x and t) by using a variant of the elementary WKB approximation.

To set this problem up mathematically we imagine our medium extending from $x = 0$ to $x = d$, and as having a refractive index $n(t)$ which is constant in space but changing in time. We describe the incident beam or pulse by saying that the wave function at the incident face $x = 0$ is $f(t)$. If we neglect the reflections at $x = 0$ and $x = d$ (these just produce inessential complications) and treat the medium as non dispersive, then the wave function $\psi(x,t)$ in the medium is the solution of the following boundary value problem:

$$\frac{\partial^2 \psi}{\partial x^2} = \frac{1}{c^2}\frac{\partial^2}{\partial t^2}\left(n^2(t)\,\psi(x,t)\right), \tag{122}$$

$$\psi(0,t) = f(t), \tag{123}$$

$$\psi(x,t) \text{ forward-moving for } x \gg 0. \tag{124}$$

The modulated wave that we are interested in is then given by $\psi(d,t)$, the wave function at the exit face.

It is easy to reduce the equation (122) to a form involving the time only; we just take Fourier transforms with respect to x. If

$$\overline{\psi}(s,t) \equiv \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{isx} \psi(x,t)\, dx, \tag{125}$$

then

$$\frac{d^2}{dt^2}\left(n^2(t)\overline{\psi(s,t)}\right) + \frac{c^2 s^2}{n^2(t)}\left(n^2(t)\overline{\psi}(s,t)\right) = 0. \tag{126}$$

We can use the WKB method to solve this equation if $n(t)$ is in some sense slowly-varying (precisely what this means will emerge later). The result is

$$n^2(t)\,\overline{\psi}(s,t) \approx \alpha(s)\sqrt{n(t)}\; e^{is\int_0^t \frac{c}{n(t')}dt'} + \beta(s)\sqrt{n(t)}\; e^{-is\int_0^t \frac{c}{n(t')}dt'}. \tag{127}$$

We can immediately set $\beta(s)$ equal to zero because of the boundary condition (124). (This is basically a causality condition - there are to be no waves in this problem other than those arising from our input $f(t)$ at $x = 0$) Inverting (125), we can write our wave function as

$$\psi(x,t) = \frac{1}{\sqrt{2\pi}\,[n(t)]^{3/2}} \int_{-\infty}^{\infty} e^{is\left(c\int_0^t \frac{dt'}{n(t')} - x\right)} \alpha(s)\, ds. \tag{128}$$

The boundary condition (123) then gives

$$f(t) = \frac{1}{\sqrt{2\pi}\,[n(t)]^{3/2}} \int_{-\infty}^{\infty} e^{isc\int_0^t \frac{dt'}{n(t')}} \alpha(s)\, ds \quad . \tag{129}$$

These equations are so similar that we do not need to go to all the labour of finding $\alpha(S)$ and then integrating; we can just write, by inspection

$$[n(t)]^{3/2}\psi(x,t) = [n(T(x,t))]^{3/2} f(T(x,t)),$$

where

$$c\int_0^{T(x,t)} \frac{dt'}{n(t')} = c\int_0^t \frac{dt'}{n(t')} - x,$$

so that, finally, our wave function is, approximately

$$\boxed{\begin{aligned} \psi(x,t) &= \frac{[n(T(x,t))]^{3/2}}{[n(t)]^{3/2}} f(T(x,t)) \\ \text{where} \quad x &= c\int_{T(x,t)}^{t} dt'/n(t') \; . \end{aligned}} \tag{130}$$

If we ignore the slowly-varying factor $[n(T)/n(t)]^{3/2}$, this result is conceptually very simple: the light disturbance starts out from $x = 0$ at time T and propagates with speed $c/n(t)$ to the observation point (x, t). The function $T(x,t)$ is the <u>phase</u> of the wave, so we should be able to interpret it as the solution of the appropriate Hamilton-Jacobi equation. This is indeed the case: the Hamiltonian function for this problem is

$$\omega(k,t) = \frac{ck}{n(t)} \tag{131}$$

and the Hamilton-Jacobi equation is

$$\omega\left(\frac{\partial T(x,t)}{\partial x}, t\right) = \frac{c}{n(t)}\frac{\partial T(x,t)}{\partial x} = -\frac{\partial T(x,t)}{\partial t}. \tag{132}$$

Simple differentiation shows that this equation is indeed satisfied by the $T(x,t)$ of (130). This example shows very clearly that we can define the <u>phase</u> of a wave in Hamiltonian terms without necessarily invoking the ideas of <u>wavelength or frequency</u> (Synge 1963).

We must now obtain a criterion for the validity of our result (130). Successive differentiations, and use of (132) show that the equation satisfied by our approximate solution is

$$c^2 \frac{\partial^2\psi(x,t)}{\partial x^2} = \frac{\partial^2}{\partial t^2}\left(n^2(t)\psi(x,t)\right) - \frac{(n^2\psi)}{n^{1/2}}\frac{d^2}{dt^2}(n^{1/2}),$$

which is a good approximation to (122) whenever

$$\frac{1}{n^{1/2}(t)}\frac{d^2 n^{1/2}(t)}{dt^2} \ll \frac{1}{n^2\psi}\frac{\partial^2}{\partial t^2}(n^2\psi). \tag{133}$$

In words, our result is a good approximation whenever the reflective index varies much more slowly than the wave-function; this is true for all optical situations. The actual form of $\psi(x,t)$ over long times may be quite complicated, because $T(x,t)$ may be a highly non-linear function of time even under our adiabatic conditions. However, the analytic form of $\psi(x,t)$ is the same as that of the input, $f(t)$. Basically this is because we have in this problem, no critical points which would introduce their characteristic analytic behaviour (Airy functions, etc.) into the wave function, altering it more and more from its initial form as time goes on.

It is interesting to consider what happens in the extreme non-adiabatic case, when the refractive index varies suddenly (this could be realised for instance, with sound waves in a gas). We then get a reflected wave appearing at the time t = to of the discontinuity (see fig.25). (This would not happen in quantum mechanics - there is no reflection at a "time potential step" because Schrödinger's equation is first-order in time). The reflected wave is present

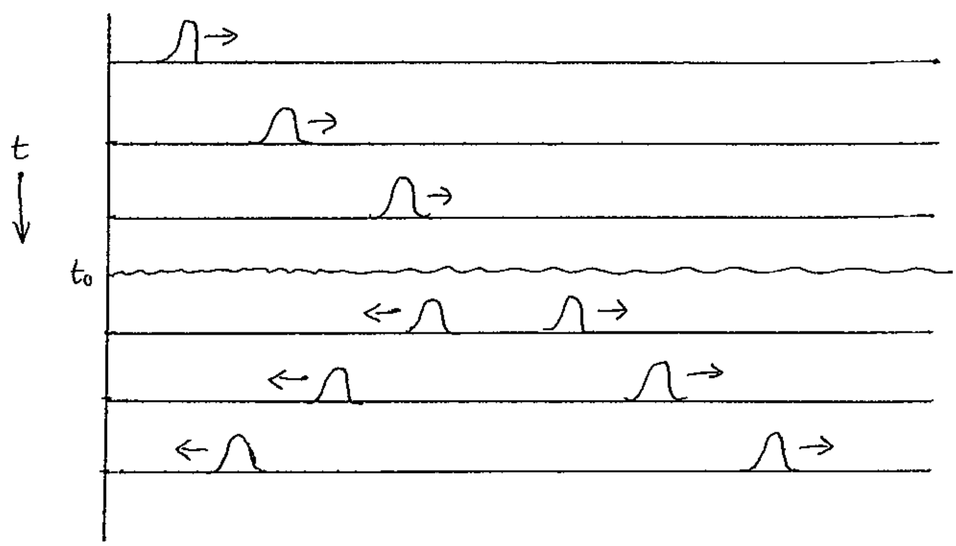

Fig.25. Reflection of a sound pulse at a time discontinuity in the density.

even when $\eta(t)$ is slowly-varying, but it has exponentially small amplitude.

Our whole problem is isomorphic to the following space-propagation situation: we have a string whose density is variable (possibly discontinuous) in space and constant in time. There are two pulses which are so arranged as to coalesce at the region of rapid density variation into a single pulse which moves along $+x$. The shape $f(x)$ of the forward-moving pulse at t = 0 is the input wave $f(t)$ of our time problem.

Now we consider the application of our result (130) to the practical problem of modulating a wave of frequency ω_0. Thus we take

$$f(t) = A \sin \omega_0 t,$$

so that, from (130)

$$\psi(d,t) \propto \sin\big(\omega_0 T(d,t)\big) \tag{134}$$

Now T (d,t) is linear over times $t-t_0$ short compared with variations in $n(t)$; but such times may still be long compared with the oscillation period $2\pi/\omega_0$ of the incident light, so we have, for times near t_0

$$\psi(d,t) \propto \sin\left(\omega_0 \frac{\partial T}{\partial t}(d,t_0)(t-t_0)\right),$$

which means that the emerging light is very nearly monochromatic, with the instantaneous frequency

$$\boxed{\omega(d,t) = \omega_0 \frac{\partial T(d,t)}{\partial t}} \tag{136}$$

Let us work out some special cases of this formula. First we take a linear increase of refractive index

$$n(t) = 1 + \alpha t.$$

From (130) we have

$$d = \frac{c}{\alpha} \ln\left(\frac{1+\alpha t}{1+\alpha T}\right)$$

or

$$T(d,t) = \frac{e^{-\alpha d/c}(1+\alpha t)}{\alpha}$$

so that the modulated frequency is

$$\omega = \omega_0 \, e^{-\alpha d/c} .$$

For this particular variation the frequency is independent of time, and decreases as the light path d increases. A second example is the exponential density increase

$$n(t) = e^{\alpha t} .$$

This leads to

$$\omega = \frac{\omega_0}{1 + \frac{\alpha d}{c} e^{\alpha t}}$$

which does depend on time.

Finally, we see what happens when the variations are <u>weak</u> as well as adiabatic - that is, we take

$$n(t) = n_0\left(1 + \varepsilon(t)\right), \tag{136}$$

where $\varepsilon(t) \ll 1$. Then

$$d = c\int_T^t \frac{dt}{n_0(1+\varepsilon(t))} \simeq \frac{c}{n_0}\left[t - T - \int_T^t \varepsilon(t')dt' + O(\varepsilon^2)\right],$$

or

$$T(d,t) = t - \frac{n_0 d}{c} - \int_{t-\frac{n_0 d}{c}}^{t} \varepsilon(t)\,dt + O(\varepsilon^2) .$$

Thus the modulated frequency is

$$\omega(d,t) \simeq \omega_0\left(1 - \varepsilon(t) + \varepsilon\left(t - \frac{n_0 d}{c}\right)\right) . \tag{137}$$

But in all practical cases involving light the time, $\frac{n_0 d}{c}$, taken for the signal to cross the container is extremely small compared with the time of significant change in $n(t)$, so that we can write

$$\omega(d,t) \simeq \omega_0 \left(1 - \frac{n_0 d}{c}\,\varepsilon(t)\right). \tag{138}$$

If the modulation of the refractive index is a sinusoid of frequency Ω, then we have

$$\varepsilon(t) = \alpha \cos \Omega t,$$

$$\omega(d,t) = \omega_0 \left(1 + \frac{\alpha n_0 d}{c}\,\Omega \sin \Omega t\right). \tag{139}$$

For a light path of 1 metre, and a frequency Ω of 3×10^3, which corresponds to speech, the amplitude of the phase modulation of the light is smaller than that of amplitude modulation of $n(t)$ by a factor $n_0 d \Omega / c \simeq 10^{-5}$, which is disappointingly small for applications to communications.

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My interest in short-wavelength phenomena was aroused by a series of lectures given in London by Professor J.L.Synge on "The Hamiltonian theory of rays and waves," in late 1964. Previously, I had been introduced to the mathematical idea of uniform asymptotic approximations by my former supervisor, Professor R.B.Dingle. The work reported here is effectively the fusion of these two conceptions; it has been carried out in Bristol with the sympathy and encouragement of Professor J.M.Ziman.

I should like to thank all three for their inspiration and help, and to acknowledge the support provided by an SRC research fellowship.

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