CHAPTER VII

THE QUASI-CLASSICAL CASE

§46. The wave function in the quasi-classical case

If the de Broglie wavelengths of particles are small in comparison with the characteristic dimensions L which determine the conditions of a given problem, then the properties of the system are close to being classical, just as wave optics passes into geometrical optics as the wavelength tends to zero.

Let us now investigate more closely the properties of *quasi-classical* systems. To do this, we make in Schrödinger's equation

$$\sum_a \frac{\hbar^2}{2m_a}\triangle_a\psi+(E-U)\psi = 0$$

the substitution

$$\psi = e^{(i/\hbar)\sigma}. \tag{46.1}$$

For the function σ we obtain the equation

$$\sum_a \frac{1}{2m_a}(\nabla_a\sigma)^2-\sum_a \frac{i\hbar}{2m_a}\triangle_a\sigma = E-U. \tag{46.2}$$

Since the system is supposed almost classical in its properties, we seek σ in the form of a series:

$$\sigma = \sigma_0+(\hbar/i)\sigma_1+(\hbar/i)^2\sigma_2+ \dots , \tag{46.3}$$

expanded in powers of $\hbar$.

We begin by considering the simplest case, that of one-dimensional motion of a single particle. Equation (46.2) then reduces to

$$\sigma'^2/2m-i\hbar\sigma''/2m = E-U(x), \tag{46.4}$$

where the prime denotes differentiation with respect to the coordinate x.

In the first approximation we write $\sigma = \sigma_0$ and omit from the equation the term containing $\hbar$:

$$\sigma_0'^2/2m = E-U(x).$$

Hence we find

$$\sigma_0 = \pm \int \sqrt{\{2m[E-U(x)]\}}\, dx.$$

The integrand is simply the classical momentum $p(x)$ of the particle, expressed as a function of the coordinate. Defining the function $p(x)$ with the + sign in front of the radical, we have

$$\sigma_0 = \pm \int p\, \mathrm{d}x, \quad p = \sqrt{[2m(E-U)]}, \tag{46.5}$$

as we should expect from the limiting expression (6.1) for the wave function.† The approximation made in equation (46.4) is legitimate only if the second term on the left-hand side is small compared with the first, i.e. we must have $\hbar|\sigma''/\sigma'^2| \ll 1$ or

$$|\mathrm{d}(\hbar/\sigma')/\mathrm{d}x| \ll 1.$$

In the first approximation we have, according to (46.5), $\sigma' = p$, so that the condition obtained can be written

$$|\mathrm{d}(\lambda/2\pi)/\mathrm{d}x| \ll 1, \tag{46.6}$$

where $\lambda(x) = 2\pi\hbar/p(x)$ is the de Broglie wavelength of the particle, expressed as a function of x by means of the classical function $p(x)$. Thus we have obtained a quantitative *quasi-classicality condition*: the wavelength of the particle must vary only slightly over distances of the order of itself. The formulae here derived are not applicable in regions of space where this condition is not satisfied.

The condition (46.6) can be written in another form by noticing that

$$\frac{\mathrm{d}p}{\mathrm{d}x} = \frac{\mathrm{d}}{\mathrm{d}x}\sqrt{[2m(E-U)]} = -\frac{m}{p}\frac{\mathrm{d}U}{\mathrm{d}x} = \frac{mF}{p},$$

where $F = -\mathrm{d}U/\mathrm{d}x$ is the classical force acting on the particle in the external field. In terms of this force we find

$$m\hbar|F|/p^3 \ll 1. \tag{46.7}$$

It is seen from this that the quasi-classical approximation becomes inapplicable if the momentum of the particle is too small. In particular, it is clearly inapplicable near *turning points*, i.e. near points where the particle, according to classical mechanics, would stop and begin to move in the opposite direction. These points are given by the equation $p(x) = 0$, i.e. $E = U(x)$. As $p \to 0$, the de Broglie wavelength tends to infinity, and hence cannot possibly be supposed small.

It must be emphasized, however, that the condition (46.6) or (46.7) alone may be insufficient for the quasi-classical approximation to be valid. The reason is that this condition has been derived from estimates of the various terms in the differential equation (46.4), the term omitted containing a higher derivative. It would be necessary, in fact, to stipulate the smallness of the

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† As is well known, $\int p\,\mathrm{d}x$ is the time-independent part of the action. The total mechanical action S of a particle is $S = -Et \pm \int p\,\mathrm{d}x$. The term $-Et$ is absent from σ_0, since we are considering a time-independent wave function ψ.

subsequent expansion terms in the solution of this equation, and this need not be ensured by the smallness of the term omitted. For example, if the solution for $\sigma(x)$ contains a term which increases almost linearly with the coordinate x, the smallness of the second derivative in the equation will not prevent this term from becoming large at sufficiently great distances. Such a situation occurs, in general, when the field extends to distances large in comparison with the characteristic length L over which it varies by an appreciable amount; see the discussion of (46.11) below. The quasi-classical approximation is then invalid for investigating the behaviour of the wave function at large distances.

Let us now calculate the next term in the expansion (46.3). The first-order terms in $\hbar$ in equation (46.4) give

$$\sigma_0'\sigma_1'+\tfrac{1}{2}\sigma_0'' = 0,$$

whence

$$\sigma_1' = -\sigma_0''/2\sigma_0' = -p'/2p.$$

Integrating, we find

$$\sigma_1 = -\tfrac{1}{2}\log p, \tag{46.8}$$

omitting the constant of integration.

Substituting this expression in (46.1) and (46.3), we find the wave function in the form

$$\psi = C_1 p^{-1/2} e^{(i/\hbar)\int p\,\mathrm{d}x} + C_2 p^{-1/2} e^{-(i/\hbar)\int p\,\mathrm{d}x}. \tag{46.9}$$

The factor $1/\sqrt{p}$ in this function has a simple interpretation. The probability of finding the particle at a point with coordinate between x and $x+\mathrm{d}x$ is given by the square $|\psi|^2$, i.e. is essentially proportional to $1/p$. This is exactly what we should expect for a "quasi-classical" particle, since, in classical motion, the time spent by a particle in the segment $\mathrm{d}x$ is inversely proportional to the velocity (or momentum) of the particle.

In the "classically inaccessible" parts of space, where $E < U(x)$, the function $p(x)$ is purely imaginary, so that the exponents are real. The general form of the solution of the wave equation in these regions is

$$\psi = \frac{C_1}{\sqrt{|p|}} e^{-(1/\hbar)\int |p|\,\mathrm{d}x} + \frac{C_2}{\sqrt{|p|}} e^{(1/\hbar)\int |p|\,\mathrm{d}x}. \tag{46.10}$$

It must, however, be borne in mind that the accuracy of the quasi-classical approximation is not such as to allow the retention in the wave function of exponentially small terms superimposed on exponentially large ones, and in this sense it is usually not permissible to retain both terms in (46.10).

Although there is, as a rule, no need to use the higher-order terms in the wave function, we shall derive the next term in the expansion (46.3), with a view to noting some aspects of the accuracy of the quasi-classical approximation.

The terms of order $\hbar^2$ in equation (46.4) give

$$\sigma_0'\sigma_2'+\tfrac{1}{2}\sigma_1'^2+\tfrac{1}{2}\sigma_1'' = 0,$$

whence (substituting (46.5) and (46.8) for σ_0 and σ_1)

$$\sigma_2' = p''/4p^2-3p'^2/8p^3.$$

Integrating (by parts in the first term) and introducing the force $F = pp'/m$, we obtain

$$\sigma_2 = \tfrac{1}{4}mF/p^3+\tfrac{1}{8}m^2\int (F^2/p^5)\,\mathrm{d}x.$$

The wave function in this approximation is of the form

$$\psi = e^{(i/\hbar)\sigma} = e^{(i/\hbar)\sigma_0+\sigma_1}(1-i\hbar\sigma_2)$$

or

$$\psi = \frac{\text{constant}}{\sqrt{p}}\left[1-\tfrac{1}{4}im\hbar F/p^3-\tfrac{1}{8}i\hbar m^2\int (F^2/p^5)\,\mathrm{d}x\right]e^{(i/\hbar)\int p\,\mathrm{d}x}. \tag{46.11}$$

The occurrence of imaginary correction terms in the coefficient of the exponential is equivalent to the presence of a similar correction in the phase of the wave function, i.e. of an addition to the integral $(1/\hbar)\int p\,\mathrm{d}x$ in its exponent. This correction is proportional to $\hbar$, i.e. is of order λ/L.

The second and third terms in the brackets in (46.11) must be small in comparison with unity. For the second term, this condition is the same as (46.7); for the third term, an estimate of the integral gives (46.7) only if F^2 tends to zero sufficiently rapidly at distances $\sim L$.

§47. Boundary conditions in the quasi-classical case

Let $x = a$ be a turning point, so that $U(a) = E$, and let $U > E$ for all $x > a$, so that the region to the right of the turning point is classically inaccessible. The wave function must be damped in this region. Sufficiently far from the turning point, it has the form

$$\psi = \frac{C}{2\sqrt{|p|}}\exp\left(-\frac{1}{\hbar}\left|\int_a^x p\,\mathrm{d}x\right|\right) \quad \text{for} \quad x > a, \tag{47.1}$$

corresponding to the first term in (46.10). To the left of the turning point, the wave function must be represented by a real combination (46.9) of two quasi-classical solutions of Schrödinger's equation:

$$\psi = \frac{C_1}{\sqrt{p}}\exp\left(\frac{i}{\hbar}\int_a^x p\,\mathrm{d}x\right)+\frac{C_2}{\sqrt{p}}\exp\left(-\frac{i}{\hbar}\int_a^x p\,\mathrm{d}x\right) \quad \text{for} \quad x < a. \tag{47.2}$$

To determine the coefficients in this combination we must follow the variation in the wave function from positive $x-a$ (where (47.1) holds) to negative $x-a$. In doing so, however, it is necessary to pass through a region near the turning point where the quasi-classical approximation is invalid, and the exact solution of Schrödinger's equation must be considered. For small $|x-a|$ we have

$$E-U(x) \approx F_0(x-a),\ F_0 = -[\mathrm{d}U/\mathrm{d}x]_{x=a} < 0; \tag{47.3}$$

that is, the problem in this region is one of movement in a homogeneous field. The exact solution of Schrödinger's equation for this problem has been found in §24, and the relation between the coefficients in (47.1) and (47.2) can be derived by comparison with the asymptotic forms (24.5) and (24.6) of this exact solution on either side of the turning point. Here it must be noted that (47.3) gives $p(x) = \sqrt{[2mF_0(x-a)]}$, so that the integral

$$\frac{1}{\hbar}\int_a^x p\,\mathrm{d}x = \frac{2}{3\hbar}\sqrt{(2mF_0)}(x-a)^{3/2}$$

is equal to the argument of the exponential in (24.5) or the sine in (24.6). In this discussion it is important that the region where the expansion (47.3) is valid and the quasi-classical region partly overlap: if the motion is quasi-classical in almost the whole of the field region (as we assume), then there exist values of $|x-a|$ small enough for the expansion (47.3) to be valid but also large enough for the quasi-classicality condition to be satisfied and for the asymptotic forms (24.5) and (24.6) to be applicable.†

There is, however, another approach that is methodologically more instructive and does not make use of the exact solution. For this, $\psi(x)$ must be formally regarded as a function of a complex variable x, and the passage from positive to negative $x-a$ must be along a path which is always sufficiently far from the point $x = a$, so that the quasi-classicality condition is formally satisfied along the whole path (A. Zwaan 1929). We then again consider values of $|x-a|$ such that the expansion (47.3) is also valid, so that the wave function (47.1) has the form

$$\psi(x) = \frac{C}{2\sqrt{(2m|F_0|)}}\frac{1}{(x-a)^{1/4}}\exp\left\{-\frac{1}{\hbar}\int_a^x \sqrt{[2m|F_0|(x-a)]}\,\mathrm{d}x\right\}. \tag{47.4}$$

Let us first examine the variation of this function on passing round the point $x = a$ from right to left along a semicircle of radius ρ in the upper half-

† The expansion (47.3) is valid for $|x-a| \ll L$, where L is the characteristic distance for variation of the field $U(x)$. The quasi-classicality condition (46.7) requires that $|x-a|^{3/2} \gg \hbar/\sqrt{(m|F_0|)}$. These two conditions are compatible, since the quasi-classicality of the motion far from the turning-point (i.e. for $|x-a| \sim L$) implies that $L^{3/2} \gg \hbar/\sqrt{(m|F_0|)}$.

plane of the complex variable x. On this semicircle,

$$x-a = \rho e^{i\phi}, \int_a^x \sqrt{(x-a)}\, dx = \tfrac{2}{3}\rho^{3/2}(\cos\tfrac{3}{2}\phi + i\sin\tfrac{3}{2}\phi),$$

the phase ϕ varying from 0 to π. The exponential factor in (47.4) at first (for $0 < \phi < \frac{2}{3}\pi$) increases in modulus, and then decreases to modulus 1. At the end of the semicircle the exponent becomes purely imaginary, equal to

$$-\frac{i}{\hbar}\int_a^x \sqrt{[2m|F_0|(a-x)]}\, dx = -\frac{i}{\hbar}\int_a^x p(x)\, dx.$$

In the coefficient of the exponential in (47.4), the change along the semicircle is

$$(x-a)^{-1/4} \to (a-x)^{-1/4}e^{-i\pi/4}.$$

Thus the whole function (47.4) becomes the second term in (47.2) with coefficient $C_2 = \frac{1}{2}Ce^{-i\pi/4}$.

The fact that by passing through the upper half-plane it is possible to determine only the coefficient C_2 in (47.2) has a simple explanation. If we follow the variation of the function (47.2) along the same semicircle in the opposite direction (from left to right), we see that at the beginning the first term rapidly becomes exponentially small in comparison with the second term. But the quasi-classical approximation does not allow us to include exponentially small terms in ψ superimposed on the large principal term, and this is why the first term in (47.2) is "lost" in the passage along the semicircle.

To determine the coefficient C_1, we must pass from right to left along a semicircle in the lower half-plane of the complex variable x. In a similar manner, we find that formula (47.4) then becomes the first term in (47.2) with coefficient $C_1 = \frac{1}{2}Ce^{i\pi/4}$.

Thus the wave function (47.1) for $x > a$ corresponds to the function

$$\psi = \frac{C}{\sqrt{p}}\cos\left(\frac{1}{\hbar}\int_a^x p\, dx + \tfrac{1}{4}\pi\right)$$

for $x < a$. This rule of correspondence may be written in a form independent of the side of the turning-point on which the classically inaccessible region lies:

$$\frac{C}{2\sqrt{|p|}}\exp\left\{-\left|\frac{1}{\hbar}\int_a^x p\, dx\right|\right\} \to \frac{C}{\sqrt{p}}\cos\left\{\left|\frac{1}{\hbar}\int_a^x p\, dx\right| - \tfrac{1}{4}\pi\right\} \qquad (47.5)$$

$$\text{for } U(x) > E \qquad\qquad \text{for } U(x) < E$$

(H. A. Kramers 1926).

Let us once again emphasize what is obvious from the proof, namely that this rule is associated with a particular boundary condition imposed on one side of the turning-point, and in this sense it can be applied only in a particular direction. The rule (47.5) is derived with the boundary condition that $\psi \to 0$ into the classically inaccessible region, and must be applied to a passage from the latter to the classically allowed region, as is shown by the arrow.†

If the classically accessible region is bounded (at $x = a$) by an infinitely high "potential wall", the boundary condition for the wave function at $x = a$ is $\psi = 0$ (see §18). The quasi-classical approximation is then valid up to the wall itself, and the wave function is

$$\left.\begin{aligned} \psi &= \frac{C}{\sqrt{p}} \sin \frac{1}{\hbar} \int_a^x p \, \mathrm{d}x \qquad \text{for} \quad x < a, \\ \psi &= 0 \qquad\qquad\qquad\qquad\quad \text{for} \quad x > a. \end{aligned}\right\} \tag{47.6}$$

§48. Bohr and Sommerfeld's quantization rule

States that belong to the discrete energy spectrum are quasi-classical for high values of the quantum number n, the ordinal number of the state, since this gives the number of nodes of the eigenfunction (see §21), and the distance between adjacent nodes is equal in order of magnitude to the de Broglie wavelength. For large n this distance is small, and the wavelength is therefore small in comparison with the dimensions of the region of the motion.

Let us derive the condition which determines the quantum energy levels in the quasi-classical case. To do this we consider a finite one-dimensional motion of a particle in a potential well; the classically accessible region $b \leqslant x \leqslant a$ is bounded by two turning points.‡

According to the rule (47.5), the boundary condition at $x = b$ gives (in the region right of this point) the wave function

$$\psi = \frac{C}{\sqrt{p}} \cos \left[\frac{1}{\hbar} \int_b^x p \, \mathrm{d}x - \tfrac{1}{4}\pi \right]. \tag{48.1}$$

† A passage in the opposite direction is meaningless in that even a small change of the wave function on the right in (47.5) may give rise to an exponentially increasing term in the function on the left.

‡ In classical mechanics, a particle in such a field would execute a periodic motion with period (time taken in moving from $x = b$ to $x = a$ and back)

$$T = 2 \int_b^a \mathrm{d}x/v = 2m \int_b^a \mathrm{d}x \, p,$$

where v is the velocity of the particle.

Applying the same rule to the region left of the point $x = a$, we obtain the same function in the form

$$\psi = \frac{C'}{\sqrt{p}} \cos\left[\frac{1}{\hbar}\int_x^a p\,\mathrm{d}x - \tfrac{1}{4}\pi\right].$$

If these two expressions are the same throughout the region, the sum of their phases (which is a constant) must be an integral multiple of π:

$$\frac{1}{\hbar}\int_b^a p\,\mathrm{d}x - \tfrac{1}{2}\pi = n\pi,$$

with $C = (-1)^n C'$. Hence

$$\frac{1}{2\pi\hbar} p\,\mathrm{d}x = n + \tfrac{1}{2} \tag{48.2}$$

where $\oint p\,\mathrm{d}x = 2\int_b^a p\,\mathrm{d}x$ is the integral taken over the whole period of the classical motion of the particle. This is the condition which determines the stationary states of the particle in the quasi-classical case. It corresponds to Bohr and Sommerfeld's quantization rule in the old quantum theory.

It is easy to see that the integer n is equal to the number of zeros of the wave function, and hence it is the ordinal number of the stationary state. For the phase of the wave function (48.1) increases from $-\frac{1}{4}\pi$ at $x = b$ to $(n+\frac{1}{4})\pi$ at $x = a$, so that the cosine vanishes n times in this range (outside the range $b \leqslant x \leqslant a$, the wave function decreases monotonically and has no zeros at a finite distance).†

As has been shown previously, the number n is large in the quasi-classical case. It must be emphasized, however, that the retention of the term $\frac{1}{2}$ added to n in (48.2) is nevertheless legitimate: to take account of the subsequent correction terms in the phase of the wave functions would give only terms $\sim\lambda/L$ on the right of (48.2), which are small in comparison with unity; see the remark at the end of §46.‡

In normalizing these wave functions, the integration of $|\psi|^2$ can be restricted to the range $b \leqslant x \leqslant a$, since outside this range ψ decreases exponentially. Since the argument of the cosine in (48.1) is a rapidly varying function, we can with sufficient accuracy replace the squared cosine by its mean value $\frac{1}{2}$.

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† Strictly speaking, the zeros should be counted by means of the exact form of the wave function near the turning points. If this is done, the result given in the text is confirmed.

‡ In some cases the exact expression for the energy levels $E(n)$ (as a function of the quantum number n), obtained from the exact Schrödinger's equation, is such that it retains its form as $n \to \infty$; examples are the energy levels in a Coulomb field, and those of a harmonic oscillator. In these cases, of course, the quantization rule (48.2), although really applicable only for large n, gives for the function $E(n)$ an expression which is the exact one.

This gives

$$\int |\psi|^2 \, dx \approx \tfrac{1}{2}C^2 \int\limits_b^a \frac{dx}{p(x)}$$

$$= \pi C^2/2m\omega = 1,$$

where $\omega = 2\pi/T$ is the frequency of the classical periodic motion. Thus the normalized quasi-classical function is

$$\psi = \sqrt{\frac{2\omega}{\pi v}} \cos\left[\frac{1}{\hbar}\int\limits_b^x p \, dx - \tfrac{1}{4}\pi\right]. \tag{48.3}$$

It must be recalled that the frequency ω is in general different for different levels, being a function of energy.

The relation (48.2) can also be interpreted in another manner. The integral $\oint p \, dx$ is the area enclosed by the closed classical phase trajectory of the particle (i.e. the curve in the px-plane, which is the phase space of the particle). Dividing this area into cells, each of area $2\pi\hbar$, we have n cells altogether; n, however, is the number of states with energies not exceeding the given value (corresponding to the phase trajectory considered). Thus we can say that, in the quasi-classical case, there corresponds to each quantum state a *cell* in phase space of area $2\pi\hbar$. In other words, the number of states belonging to the volume element $\Delta p \Delta x$ of phase space is

$$\Delta p \Delta x / 2\pi\hbar. \tag{48.4}$$

If we introduce, instead of the momentum, the *wave number* $k = p/\hbar$, this number can be written

$$\Delta k \Delta x / 2\pi.$$

It is, as we should expect, the same as the familiar expression for the number of characteristic vibrations of a wave field (see *Fields*, §52).

Starting from the quantization rule (48.2), we can ascertain the general nature of the distribution of levels in the energy spectrum. Let ΔE be the distance between two neighbouring levels, i.e. levels whose quantum numbers n differ by unity. Since ΔE is small (for large n) compared with the energy itself of the levels, we can write, from (48.2),

$$\Delta E \oint (\partial p/\partial E) \, dx = 2\pi\hbar.$$

But $\partial E/\partial p = v$, so that

$$\oint (\partial p/\partial E) \, dx = \oint dx/v = T.$$

Hence we have

$$\Delta E = 2\pi\hbar/T = \hbar\omega. \tag{48.5}$$

Thus the distance between two neighbouring levels is $\hbar\omega$. The frequencies ω may be regarded as approximately the same for several adjacent levels (the difference in whose numbers n is small compared with n itself). Hence we reach the conclusion that, in any small range of a quasi-classical part of the spectrum, the levels are equidistant, at intervals of $\hbar\omega$. This result could have been foreseen, since, in the quasi-classical case, the frequencies corresponding to transitions between different energy levels must be integral multiples of the classical frequency ω.

It is of interest to investigate what the matrix elements of any physical quantity f become in the limit of classical mechanics. To do this, we start from the fact that the mean value $\bar{f}$ in any quantum state must become, in the limit, simply the classical value of the quantity, provided that the state itself gives, in the limit, a motion of the particle in a definite path. A wave packet (see §6) corresponds to such a state; it is obtained by superposition of a number of stationary states with nearly the same energy. The wave function of such a state is of the form

$$\Psi = \sum_n a_n \Psi_n,$$

where the coefficients a_n are noticeably different from zero only in some range Δn of values of the quantum number n such that $1 \ll \Delta n \ll n$; the numbers n are supposed large, because the stationary states are quasi-classical. The mean value of f is, by definition,

$$\bar{f} = \int \Psi^* \hat{f} \Psi \, dx = \sum_n \sum_m a_m^* a_n f_{mn} e^{i\omega_{mn}t},$$

or, replacing the summation over n and m by a summation over n and the difference $m - n = s$,

$$\bar{f} = \sum_n \sum_s a_{n+s}^* a_n f_{n+s,n} e^{i\omega st},$$

where we have put $\omega_{mn} = s\omega$ in accordance with (48.5).

The matrix elements f_{nm} calculated by means of the quasi-classical wave functions decrease rapidly in magnitude as the difference $m-n$ increases, though at the same time they vary only slowly with n itself ($m-n$ being fixed). Hence we can write approximately

$$\bar{f} = \sum_n \sum_s a_n^* a_n f_s e^{i\omega st} = \sum_n |a_n|^2 \sum_s f_s e^{i\omega st},$$

where we have introduced the notation $f_s = f_{\bar{n}+s,\bar{n}}$, $\bar{n}$ being some mean value of the quantum number in the range Δn. But $\sum |a_n|^2 = 1$; hence

$$\bar{f} = \sum_s f_s e^{i\omega st}.$$

The sum obtained is in the form of an ordinary Fourier series. Since $\bar{f}$ must, in the limit, coincide with the classical quantity $f(t)$, we arrive at the result that the matrix elements f_{mn} in the limit become the components f_{m-n} in the expansion of the classical function $f(t)$ as a Fourier series.

Similarly, the matrix elements for transitions between states of the continuous spectrum become the components in the expansion of $f(t)$ as a Fourier integral. Here the wave functions of the stationary states must be normalized by $(1/\hbar)$ times the delta function of energy.

All the above results can be generalized immediately to systems with several degrees of freedom, executing a finite motion for which the problem in classical mechanics allows a complete separation of the variables in the Hamilton–Jacobi method (called a *conditionally periodic* motion; see *Mechanics*, §52). After separation of the variables for each degree of freedom, the problem reduces to a one-dimensional problem, and the corresponding quantization conditions are

$$\oint p_i \,\mathrm{d}q_i = 2\pi\hbar(n_i+\gamma_i), \tag{48.6}$$

where the integral is taken over the period of variation of the generalized coordinate q_i, and γ_i is a number of the order of unity which depends on the nature of the boundary conditions for the degree of freedom considered.†

In the general case of an arbitrary (not conditionally periodic) motion in several dimensions the formulation of the quasi-classical conditions of quantization calls for more far-reaching considerations.‡ The concept of "cells" in phase space is, however, applicable (in the quasi-classical approximation) in the same form always. This is clear from the above-mentioned relationship between it and the number of characteristic vibrations of the wave field in a given volume of space. In the general case of a system with s degrees of freedom, there are

$$\Delta N = \Delta q_1 \dots \Delta q_s \Delta p_1 \dots \Delta p_s/(2\pi\hbar)^s \tag{48.7}$$

quantum states in a volume element in phase space.||

PROBLEMS

PROBLEM 1. Determine (approximately) the number of discrete energy levels of a particle moving in an arbitrary (not central) field $U(\mathbf{r})$ which satisfies the quasi-classical condition.

SOLUTION. The number of states belonging to a volume of phase space which corresponds to momenta in the range $0 \leqslant p \leqslant p_{\max}$ and particle coordinates in the volume element $\mathrm{d}V$

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† For example, in motion in a centrally symmetric field we have

$$\oint p_r \,\mathrm{d}r = 2\pi\hbar(n_r+\tfrac{1}{2}), \quad \oint p_\theta \,\mathrm{d}\theta = 2\pi\hbar(l-m+\tfrac{1}{2}), \quad \oint p_\phi \,\mathrm{d}\phi = 2\pi\hbar m,$$

where $n_r = n-l-1$ is the radial quantum number. The last of the three equations simply expresses the fact that p_ϕ is the z-component of the angular momentum, equal to $\hbar m$.

‡ See J. B. Keller, *Annals of Physics* **4**, 180, 1958.

|| In particular, for one particle, $\mathrm{d}^3p/(2\pi\hbar)^3$ is the number of states for a range d^3p of values of the momentum in unit volume of coordinate space. This explains the agreement of the two methods of normalizing the plane wave (15.8), mentioned in the footnote to that formula.

is $\frac{4}{3}\pi p_{\max}^3\, \mathrm{d}V/(2\pi\hbar)^3$. For given $\mathbf{r}$ the particle can have (in its classical motion) a momentum satisfying the condition $E = p^2/2m + U(\mathbf{r}) \leqslant 0$. Substituting $p_{\max} = \sqrt{[-2mU(\mathbf{r})]}$, we obtain the total number of states of the discrete spectrum:

$$\frac{\sqrt{2}}{3\pi^2}\frac{m^{3/2}}{\hbar^3}\int(-U)^{3/2}\,\mathrm{d}V,$$

where the integration is over the region of space in which $U < 0$. This integral diverges (i.e. the number of states is infinite) if U decreases at infinity as r^{-s} with $s < 2$, in accordance with the results of §18.

Problem 2. The same as Problem 1, but for a quasi-classical centrally symmetric field $U(r)$ (V. L. Pokrovskiĭ).

Solution. In a centrally symmetric field the number of states is not the same as the number of energy levels, on account of the degeneracy of the latter with respect to the direction of the angular momentum. The required number can be found by noting that the number of levels with a given value of the angular momentum M is the same as the number of (non-degenerate) levels for a one-dimensional motion in a field with potential energy $U_{\text{eff}} = U(r)+M^2/2mr^2$. The maximum possible value of the momentum p_r for given r and energies $E \leqslant 0$ is $p_{r,\max} = \sqrt{(-2mU_{\text{eff}})}$. The number of states (i.e. the required number of levels) is therefore

$$\int\frac{\mathrm{d}r\,\mathrm{d}p_r}{2\pi\hbar} = \frac{\sqrt{(2m)}}{2\pi\hbar}\int\sqrt{\left(-U-\frac{M^2}{2mr^2}\right)}\,\mathrm{d}r.$$

The required total number of discrete levels is obtained from this by integration with respect to $M/\hbar$ (which replaces in the quasi-classical case the summation with respect to l), and is

$$(m/4\hbar^2)\int(-U)r\,\mathrm{d}r.$$

§49. Quasi-classical motion in a centrally symmetric field

In motion in a centrally symmetric field the wave function of a particle falls, as we know, into an angular and a radial part. Let us first consider the former.

The dependence of the angular wave function on the angle ϕ (determined by the quantum number m) is so simple that the question of finding approximate formulae for it does not arise. The dependence on the polar angle θ is, according to the general rule, quasi-classical if the corresponding quantum number l is large (this condition will be more precisely formulated below).

We shall here confine ourselves to deriving the quasi-classical expression for the angular function for the case (the most important one in applications) of states whose magnetic quantum number is zero ($m = 0$).† This function is, apart from a constant factor, the Legendre polynomial $P_l(\cos\theta)$ (see (28.8)), and satisfies the differential equation

$$\mathrm{d}^2P_l/\mathrm{d}\theta^2+\cos\theta\,\mathrm{d}P_l/\mathrm{d}\theta+l(l+1)P_l = 0. \tag{49.1}$$

The substitution

$$P_l(\cos\theta) = \chi(\theta)/\sqrt{\sin\theta} \tag{49.2}$$

† The opposite case, $m = l$, must correspond in the limit to motion in a classical orbit lying in the equatorial plane $\theta = \frac{1}{2}\pi$, since $P_l^l(\cos\theta) = \text{constant} \times \sin^l\theta$, and as $l \to \infty$ this function (and therefore $|\psi|^2$) tends to zero for all $\theta \neq \frac{1}{2}\pi$.

reduces this to

$$\chi''+[(l+\tfrac{1}{2})^2+\tfrac{1}{4}\operatorname{cosec}^2\theta]\chi = 0, \tag{49.3}$$

which does not contain the first derivative and is similar in appearance to the one-dimensional Schrödinger's equation.

In equation (49.3), the part of the de Broglie wavelength is played by

$$\lambda = 2\pi\,[(l+\tfrac{1}{2})^2+\tfrac{1}{4}\operatorname{cosec}^2\theta]^{-1/2}.$$

The requirement that the derivative $\mathrm{d}(\lambda/2\pi)/\mathrm{d}x$ is small (the condition (46.6)) gives the inequalities

$$\theta l \gg 1, \qquad (\pi-\theta)l \gg 1, \tag{49.4}$$

which are the conditions that the angular part of the wave function is quasi-classical. For large l these conditions hold for almost all values of θ, excluding only a range of angles very close to 0 or π.

When the conditions (49.4) are satisfied, we can neglect the second term in the brackets in (49.3) compared with the first:

$$\chi''+(l+\tfrac{1}{2})^2\chi = 0.$$

The solution of this equation is

$$\chi = \sqrt{\sin\theta}\,P_l(\cos\theta) = A\sin[(l+\tfrac{1}{2})\theta+\alpha], \tag{49.5}$$

where A and α are constants.

For angles $\theta \ll 1$, we can put in equation (49.1) $\cos\theta \approx 1/\theta$; replacing also $l(l+1)$ by the approximation $(l+\frac{1}{2})^2$, we obtain the equation

$$\frac{\mathrm{d}^2P_l}{\mathrm{d}\theta^2}+\frac{1}{\theta}\frac{\mathrm{d}P_l}{\mathrm{d}\theta}+(l+\tfrac{1}{2})^2P_l = 0,$$

which has as solution the Bessel function of zero order:

$$P_l(\cos\theta) = J_0[(l+\tfrac{1}{2})\theta], \quad \theta \ll 1. \tag{49.6}$$

The constant factor is put equal to unity, since we must have $P_l = 1$ for $\theta = 0$. The approximate expression (49.6) for P_l is valid for all angles $\theta \ll 1$. In particular, it can be applied for angles in the range $1/l \ll \theta \ll 1$, where it must agree with the expression (49.5), which holds for all $\theta \gg 1/l$. For $\theta l \gg 1$ the Bessel function can be replaced by its asymptotic expression for large values of the argument, and we obtain

$$P_l \approx \sqrt{\frac{2}{\pi l}}\frac{\sin[(l+\frac{1}{2})\theta+\frac{1}{4}\pi]}{\sqrt{\theta}}$$

(we can neglect $\frac{1}{2}$ in the coefficient compared with l). On comparison with (49.5), we find that $A = \sqrt{(2/\pi l)}$, $\alpha = \frac{1}{4}\pi$. Thus we obtain finally the following expression for $P_l(\cos\theta)$, applicable in the quasi-classical case:†

$$P_l(\cos\theta) \approx \sqrt{\frac{2}{\pi l}}\frac{\sin[(l+\frac{1}{2})\theta+\frac{1}{4}\pi]}{\sqrt{\sin\theta}}. \tag{49.7}$$

The normalized spherical harmonic function Y_{l0} is obtained from this as (cf. (28.8))

$$Y_{l0} \approx \frac{i^l}{\pi}\frac{\sin[(l+\frac{1}{2})\theta+\frac{1}{4}\pi]}{\sqrt{\sin\theta}}. \tag{49.8}$$

Let us now turn to the radial part of the wave function. It has been shown in §32 that the function $\chi(r) = rR(r)$ satisfies an equation identical with the one-dimensional Schrödinger's equation, with the potential energy

$$U_l(r) = U(r)+\frac{\hbar^2}{2m}\frac{l(l+1)}{r^2}.$$

Hence we can apply the results obtained in the previous sections, if the potential energy is understood to be the function $U_l(r)$.

The case $l = 0$ is the simplest. The centrifugal energy vanishes and, if the field $U(r)$ satisfies the necessary condition (46.6), the radial wave function will be quasi-classical in all space. For $r = 0$ we must have $\chi = 0$, and hence the quasi-classical function $\chi(r)$ is determined by formulae (47.6).

If $l \neq 0$, the centrifugal energy also must satisfy the condition (46.6). In the region of small r, where the centrifugal energy is of the same order as the total energy, the wavelength $\lambda = 2\pi\hbar/p \sim r/l$, and the condition (46.6) gives $l \gg 1$. Thus, if l is small, the quasi-classical condition is violated by the centrifugal energy in the region of small r. It is easily seen that we obtain the correct value of the phase of the quasi-classical wave function $\chi(r)$ by calculating it from the formulae for one-dimensional motion, replacing the coefficient $l(l+1)$ in the potential energy $U_l(r)$ by $(l+\frac{1}{2})^2$:‡

$$U_l(r) = U(r)+\frac{\hbar^2}{2m}\frac{(l+\frac{1}{2})^2}{r^2}. \tag{49.9}$$

The question of the applicability of the quasi-classical approximation to a Coulomb field $U = \pm\alpha/r$ requires special consideration. The most important part of the whole region of the motion is that corresponding to distances r for which $|U| \sim |E|$, i.e. $r \sim \alpha/|E|$. The condition for quasi-classical motion in this region amounts to the requirement that the wavelength $\lambda \sim \hbar/\sqrt{(2m|E|)}$ is small compared with the dimensions $\alpha/|E|$ of the

† Note that, as a result of replacing $l(l+1)$ by $(l+\frac{1}{2})^2$, we have obtained an expression which is multiplied by $(-1)^l$ when θ is replaced by $\pi-\theta$; this is as it should be for the function $P_l(\cos\theta)$.

‡ For example, in the simple case of free motion ($U = 0$) the phase of the function calculated from formula (48.1) with U_l from (49.9) will be the same as the phase of (33.12) for large r, as it should be.

region; this gives

$$|E| \ll m\alpha^2/\hbar^2, \tag{49.10}$$

i.e. the absolute value of the energy must be small compared with the energy of the particle in the first Bohr orbit. This condition can also be written in the form

$$\alpha/\hbar v \gg 1, \tag{49.11}$$

where $v \sim \sqrt{(|E|/m)}$ is the velocity of the particle. It should be noticed that this condition is the opposite of the condition (45.7) for the applicability of perturbation theory to a Coulomb field.

The region of small distances ($|U(r)| \gg E$) is without interest in a repulsive Coulomb field, since for $U > E$ the quasi-classical wave functions diminish exponentially. In an attractive field, however, when l is small it is possible for the particle to penetrate into the region where $|U| \gg E$, so that we have to consider the limits of applicability of the quasi-classical approximation in this case. We use the general condition (46.7), putting there

$$F = -\mathrm{d}U/\mathrm{d}r = -\alpha/r^2, \quad p \approx \sqrt{(2m|U|)} \sim \sqrt{(m\alpha/r)}.$$

As a result, we find that the region of applicability of the quasi-classical approximation is restricted to distances such that

$$r \gg \hbar^2/m\alpha, \tag{49.12}$$

i.e. distances large in comparison with the "radius" of the first Bohr orbit.

PROBLEM

Determine the behaviour of the wave function near the origin, if the field becomes infinite as $\pm\alpha/r^s$, with $s > 2$, when $r \to 0$.

SOLUTION. For sufficiently small r, the wavelength $\lambda \sim \hbar/\sqrt{(m|U|)} \sim \hbar r^{s/2}/\sqrt{(m\alpha)}$, so that $\mathrm{d}\lambda/\mathrm{d}r \sim \hbar r^{s/2-1}/\sqrt{(m\alpha)} \ll 1$; thus the quasi-classical condition is satisfied. In an attractive field $U_l \to -\infty$ when $r \to 0$. The region near the origin is in this case classically accessible, and the radial wave function $\chi \sim 1/\sqrt{p}$, whence

$$\psi \sim r^{s/4-1}.$$

In a repulsive field, the region of small r is classically inaccessible. In this case the wave function tends exponentially to zero as $r \to 0$. Omitting the coefficient of the exponential function, we have

$$\psi \sim \exp\left[-\frac{1}{\hbar}\int_{r_0}^{r} p\,\mathrm{d}r\right], \text{ or } \psi \sim \exp\left\{-\frac{2\sqrt{(2m\alpha)}}{(s-2)\hbar}r^{-(s/2-1)}\right\}.$$

§50. Penetration through a potential barrier

Let us consider the motion of a particle in a field of the type shown in Fig. 13, characterized by the presence of a *potential barrier*, i.e. a region in which the potential energy $U(x)$ exceeds the total energy E of the particle. In classical mechanics, a potential barrier is "impenetrable" to a particle; in quantum mechanics, however, a particle can pass "through the barrier":

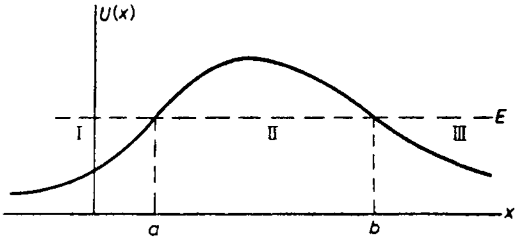

FIG. 13

the probability of this is not zero. The phenomenon is also called the *tunnel effect*.† If the field $U(x)$ satisfies the quasi-classical conditions, the transmission coefficient for the barrier can be calculated in a general form. We may remark that, in particular, these conditions give the result that the barrier must be "wide", and hence the transmission coefficient is small in the quasi-classical case.

In order not to interrupt the subsequent calculations, we shall first solve the following problem. Let the quasi-classical wave function in the region to the right of the turning point $x = b$ (where $U(x) < E$) have the form of a travelling wave:

$$\psi = \frac{C}{\sqrt{p}} \exp\left[\frac{i}{\hbar}\int\limits_b^x p\,\mathrm{d}x + \tfrac{1}{4}i\pi\right]. \tag{50.1}$$

We require to find the wave function of this state in the region $x < b$. This can be done by the same procedure as in §47, using the plane of the complex variable x. Putting

$$E - U(x) \approx F_0(x-b),\ F_0 > 0,$$

we can write the function (50.1) as

$$\psi(x) = \frac{C}{\sqrt{(2mF_0)}}\frac{1}{(x-b)^{1/4}}\exp\left\{\frac{i}{\hbar}\sqrt{(2mF_0)}\int\limits_b^x \sqrt{(x-b)}\,\mathrm{d}x + \tfrac{1}{4}i\pi\right\},$$

and pass from right to left along a semicircle in the upper half-plane:

$$x - b = \rho e^{i\phi},\ i\int\limits_b^x \sqrt{(x-b)}\,\mathrm{d}x = \tfrac{2}{3}\rho^{3/2}(-\sin\tfrac{3}{2}\phi + i\cos\tfrac{3}{2}\phi),$$

the phase ϕ varying from 0 to π. The function $\psi(x)$ at first decreases and then

† An example of this type has already occurred in §25, Problem 2.

increases in modulus, its value at the end of the semicircle being

$$\psi(x) = \frac{C}{\sqrt{(2mF_0)}}\frac{1}{(b-x)^{1/4}e^{i\pi/4}}\exp\left\{\frac{1}{\hbar}\int_x^b \sqrt{[2mF_0(x-b)]}\,\mathrm{d}x+\tfrac{1}{4}i\pi\right\}.$$

Thus we obtain the correspondence rule†

$$\frac{C}{\sqrt{p}}\exp\left\{\frac{i}{\hbar}\int_b^x p\,\mathrm{d}x+\tfrac{1}{4}i\pi\right\} \to \frac{C}{\sqrt{|p|}}\exp\left\{\frac{1}{\hbar}\left|\int_b^x p\,\mathrm{d}x\right|\right\}. \tag{50.2}$$

$$\text{for } x > b \qquad\qquad\qquad \text{for } x < b$$

It must be emphasized that this rule presupposes a particular form of the wave function (a wave travelling to the right) in the classically allowed region, and must be applied to go from the latter to the classically inaccessible region.

Let us now go on to calculate the coefficient for the penetration of the potential barrier. Let the particle be incident on the barrier from left to right, coming from region I. Then, in region III beyond the barrier, there will be only the wave that has passed through the barrier and is propagated to the right; the wave function in this region may be written

$$\psi = \sqrt{\frac{D}{v}}\exp\left(\frac{i}{\hbar}\int_b^x p\,\mathrm{d}x+\tfrac{1}{4}i\pi\right), \tag{50.3}$$

where $v = p/m$ is the particle velocity and D the current density in the wave. Using the rule (50.2), we can now find the wave function in region II, within the barrier:

$$\begin{aligned}\psi &= \sqrt{\frac{D}{|v|}}\exp\left(\frac{1}{\hbar}\left|\int_x^b p\,\mathrm{d}x\right|\right)\\ &= \sqrt{\frac{D}{|v|}}\exp\left(\frac{1}{\hbar}\left|\int_a^b p\,\mathrm{d}x\right|-\frac{1}{\hbar}\left|\int_a^x p\,\mathrm{d}x\right|\right).\end{aligned} \tag{50.4}$$

† In a passage from right to left through the lower half-plane, the function $\psi(x)$ at first increases and then decreases in modulus, becoming an exponentially small quantity on the left-hand axis ($\phi \to -\pi$), which it would not be legitimate to keep superimposed on the exponentially large function (50.2). In the region where $\psi(x)$ is exponentially large, the inexactness of the quasi-classical approximation loses the exponentially small correction which for $\phi \to -\pi$ could become an exponentially large term, and the latter is therefore lost also.

Finally, applying the rule (47.5), we have in region I in front of the barrier

$$\psi = 2\sqrt{\frac{D}{v}}\exp\left(\frac{1}{\hbar}\int_a^b |p|\,dx\right)\cos\left(\frac{1}{\hbar}\int_x^a p\,dx - \tfrac{1}{4}\pi\right).$$

If we put here

$$D = \exp\left(-\frac{2}{\hbar}\int_a^b |p|\,dx\right), \tag{50.5}$$

this becomes

$$\psi = \frac{2}{\sqrt{v}}\cos\left(\frac{1}{\hbar}\int_a^x p\,dx + \tfrac{1}{4}\pi\right)$$

$$= \frac{1}{\sqrt{v}}\exp\left(\frac{i}{\hbar}\int_a^x p\,dx + \tfrac{1}{4}i\pi\right) + \frac{1}{\sqrt{v}}\exp\left(-\frac{i}{\hbar}\int_a^x p\,dx - \tfrac{1}{4}i\pi\right).$$

This first term (which becomes a plane wave $\psi = e^{(i/\hbar)px}$ as $x \to -\infty$) represents a wave incident on the barrier, and the second a reflected wave. The normalization chosen corresponds to a unit current density in the incident wave, and therefore D, the current density in the transmitted wave, is equal to the required transmission coefficient for the barrier. Note that this formula is applicable only if the exponent is large, so that D itself is small.†

It has been assumed in the foregoing that the field $U(x)$ satisfies the quasi-classical condition over the whole extent of the barrier (excluding only the immediate neighbourhood of the turning points). In practice, however, we often have to deal with barriers where the potential energy curve on one side drops so steeply that the quasi-classical approximation is inapplicable. The exponential factor in D remains the same in this case as in formula (50.5), but the coefficient of the exponential (equal to unity in (50.5)) is different. To calculate it we must, essentially, calculate the exact wave function in the non-quasi-classical region and determine the quasi-classical wave function inside the barrier in accordance with this.

PROBLEMS

PROBLEM 1. Determine the transmission coefficient for the potential barrier shown in Fig. 14 (p. 182): $U(x) = 0$ for $x < 0$, $U(x) = U_0 - Fx$ for $x > 0$; only the exponential factor need be calculated.

† The exponential smallness of D is related to the fact that the amplitudes of the incident and reflected waves in region I are found to be the same; the exponentially small difference between them is lost in the quasi-classical approximation.

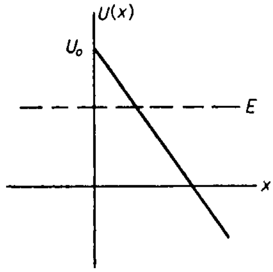

FIG. 14

SOLUTION. A simple calculation gives the result

$$D \sim \exp\left\{-\frac{4\sqrt{(2m)}}{3\hbar F}(U_0-E)^{3/2}\right\}.$$

PROBLEM 2. Determine the probability that a particle (with zero angular momentum) will emerge from a centrally symmetric potential well with $U(r) = -U_0$ for $r < r_0$, $U(r) = \alpha/r$ for $r > r_0$ (Fig. 15).†

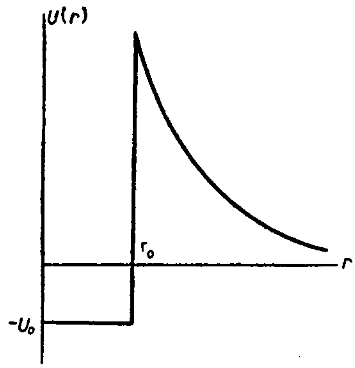

FIG. 15

SOLUTION. The centrally symmetric problem reduces to a one-dimensional one, so that the formulae obtained above can be applied. We have

$$w \sim \exp\left\{-\frac{2}{\hbar}\int\limits_{r_0}^{\alpha/E}\sqrt{\left[2m\left(\frac{\alpha}{r}-E\right)\right]}\,dr\right\}.$$

Evaluating the integral, we finally obtain

$$w \sim \exp\left\{-\frac{2\alpha}{\hbar}\sqrt{\frac{2m}{E}}\left[\cos^{-1}\sqrt{\frac{Er_0}{\alpha}}-\sqrt{\left\{\frac{Er_0}{\alpha}\left(1-\frac{Er_0}{\alpha}\right)\right\}}\right]\right\}.$$

In the limiting case $r_0 \to 0$, this formula becomes

$$w \sim e^{-(\pi\alpha/\hbar)\sqrt{(2m/E)}} = e^{-2\pi\alpha/\hbar v}.$$

These formulae are applicable when the exponent is large, i.e. when $\alpha/\hbar v \gg 1$. This condition agrees, as it should, with the condition (49.11) for quasi-classical motion in a Coulomb field.

† This problem was first discussed by G. Gamow (1928) and by R. W. Gurney and E. U. Condon (1929) in connection with the theory of radioactive α-decay.

Problem 3. The field $U(x)$ consists of two symmetrical potential wells (I and II in Fig. 16), separated by a barrier. If the barrier were impenetrable to a particle, there would be energy levels corresponding to the motion of the particle in one or other well, the same for both wells. The fact that a passage through the barrier is possible results in a splitting of each of these levels into two neighbouring ones, corresponding to states in which the particle moves simultaneously in both wells. Determine the magnitude of the splitting (the field $U(x)$ is supposed quasi-classical).

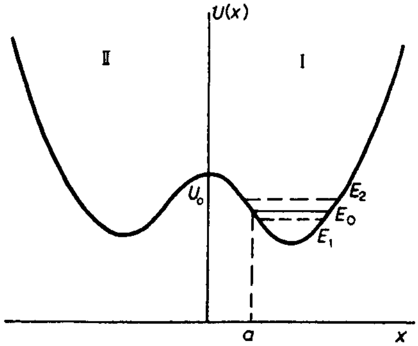

Fig. 16

Solution. An approximate solution of Schrödinger's equation in the field $U(x)$, neglecting the probability of passage through the barrier, can be constructed with the quasi-classical wave function $\psi_0(x)$ which describes the motion with a certain energy E_0 in one well, say I, i.e. which is exponentially damped on both sides of this well; the function $\psi_0(x)$ is assumed to be normalized so that the integral of $\psi_0{}^2$ over well I is unity. When the small probability of tunnelling is taken into account, the level E_0 splits into levels E_1 and E_2. The correct zero-approximation wave functions corresponding to these levels are the symmetric and antisymmetric combinations of $\psi_0(x)$ and $\psi_0(-x)$:

$$\left.\begin{aligned} \psi_1(x) &= \frac{1}{\sqrt{2}}[\psi_0(x)+\psi_0(-x)], \\ \psi_2(x) &= \frac{1}{\sqrt{2}}[\psi_0(x)-\psi_0(-x)]. \end{aligned}\right\} \quad (1)$$

In well I, the function $\psi_0(-x)$ is vanishingly small in comparison with $\psi_0(x)$; in well II the opposite is true. The product $\psi_0(x)\psi_0(-x)$ is therefore vanishingly small everywhere, and the functions (1) are normalized so that the integrals of their squares over wells I and II are unity.

Schrödinger's equations are

$$\psi_0''+(2m/\hbar^2)(E_0-U)\psi_0 = 0, \quad \psi_1''+(2m/\hbar^2)(E_1-U)\psi_1 = 0;$$

we multiply the former by ψ_1 and the latter by ψ_0, subtract corresponding terms, and integrate over x from 0 to ∞. Bearing in mind that, for $x = 0$, $\psi_1 = \sqrt{2}\psi_0$ and $\psi_1' = 0$, and that

$$\int_0^\infty \psi_0\psi_1\, dx \approx \frac{1}{\sqrt{2}}\int_0^\infty \psi_0{}^2\, dx = 1/\sqrt{2},$$

we find

$$E_1-E_0 = -(\hbar^2/m)\psi_0(0)\psi_0'(0).$$

Similarly, we find for E_2-E_0 the same expression with the sign changed. Thus

$$E_2-E_1 = (2\hbar^2/m)\psi_0(0)\psi_0'(0).$$

By means of formula (47.1), with the coefficient C from (48.3), we find that

$$\psi_0(0) = \sqrt{\frac{\omega}{2\pi v_0}}\exp\left[-\frac{1}{\hbar}\int_0^a |p|\,dx\right], \quad \psi_0'(0) = \frac{mv_0}{\hbar}\psi_0(0),$$

where $v_0 = \sqrt{[2(U_0-E_0)/m]}$. Thus

$$E_2-E_1 = \frac{\omega\hbar}{\pi}\exp\left[-\frac{1}{\hbar}\int_{-a}^{a}|p|\,dx\right].$$

where a is the turning point corresponding to the energy E_0; see Fig. 16.

PROBLEM 4. Determine the exact value of the transmission coefficient D for the passage of a particle through a parabolic potential barrier $U(x) = -\frac{1}{2}kx^2$ (supposing that D is *not* small) (E. C. Kemble 1935).†

SOLUTION. Whatever the values of k and E, the motion is quasi-classical at sufficiently large distances $|x|$, with

$$p = \sqrt{[2m(E+\tfrac{1}{2}kx^2)]} \approx x\sqrt{(mk)}+E\sqrt{(m/k)}/x,$$

and the asymptotic form of the solutions of Schrödinger's equation is

$$\psi = \text{constant}\times e^{\pm i\xi^2/2}\xi^{\pm i\epsilon-1/2},$$

where we have introduced the notation

$$\xi = x(mk/\hbar^2)^{1/4}, \qquad \epsilon = (E/\hbar)\sqrt{(m/k)}.$$

We are interested in the solution which, as $x \to +\infty$, contains only a wave which has passed the barrier, i.e. is propagated from left to right. We put

$$\text{as } x \to \infty, \quad \psi = Be^{i\xi^2/2}\xi^{i\epsilon-1/2}, \tag{1}$$

$$\text{as } x \to -\infty, \quad \psi = e^{-i\xi^2/2}(-\xi)^{-i\epsilon-1/2}+Ae^{i\xi^2/2}(-\xi)^{i\epsilon-1/2}. \tag{2}$$

In the expression (2), the first term represents the incident wave, and the second the reflected wave (the direction of propagation of a wave is that in which its phase increases). The relation between A and B can be found by using the fact that in this case the asymptotic expression for ψ is valid in the whole of a sufficiently distant region of the plane of the complex variable ξ. Let us follow the variation of the function (1) as we go round a semicircle of large radius ρ in the upper half-plane of ξ:

$$\xi = \rho e^{i\phi}, i\xi^2 = \rho^2(-\sin 2\phi + i\cos 2\phi),$$

with ϕ varying from 0 to π. As a result of traversing this semicircle, the function (1) becomes the second term in (2), with coefficient

$$A = B(e^{i\pi})^{i\epsilon-1/2} = -iBe^{-\pi\epsilon}; \tag{3}$$

in the part of the path ($\frac{1}{2}\pi < \phi < \pi$) where the modulus $|e^{i\xi^2/2}|$ is exponentially large, the exponentially small quantity which should give the first term in (2) is lost.‡

† The solution of this problem can also be applied to penetration sufficiently near the top of any barrier $U(x)$ whose dependence on x near the maximum is quadratic.

‡ The passage through the lower half-plane to determine A would be unsuitable, since on the part of the path ($-\pi < \phi < -\frac{1}{2}\pi$) that adjoins its left-hand end (where ψ is given by (2)), the term in $e^{i\xi^2/2}$ is exponentially small in comparison with $e^{-i\xi^2/2}$.

With the normalization of the incident wave chosen in (2), the condition of conservation of number of particles is

$$|A|^2+|B|^2 = 1. \tag{4}$$

From (3) and (4) we find the required transmission coefficient:

$$D = |B|^2 = 1/(1+e^{-2\pi\epsilon}).$$

This formula holds for any E. If the energy is large and negative, it gives $D \approx e^{-2\pi|\epsilon|}$ in accordance with formula (50.5). For $E > 0$, the quantity

$$R = 1-D = 1/(1+e^{2\pi\epsilon})$$

is the coefficient of reflection above the barrier.

§51. Calculation of the quasi-classical matrix elements

A direct calculation of the matrix elements of any physical quantity f with respect to the quasi-classical wave functions presents great difficulty. We may suppose that the energies of the states between which the matrix element is calculated are not close to each other, so that the element does not reduce to the Fourier component of the quantity f (§48). The difficulties arise because, owing to the fact that the wave functions are exponential (with a large imaginary exponent), the integrand oscillates rapidly.

We shall consider a one-dimensional case (motion in a field $U(x)$), and suppose for simplicity that the operator of the physical quantity is merely a function $f(x)$ of the coordinate. Let ψ_1 and ψ_2 be the wave functions corresponding to some values E_1 and E_2 of the energy of the particle (with $E_2 > E_1$, Fig. 17); we shall suppose that ψ_1 and ψ_2 are taken real. We have to calculate the integral

$$f_{12} = \int_{-\infty}^{\infty} \psi_1 f \psi_2 \, dx. \tag{51.1}$$

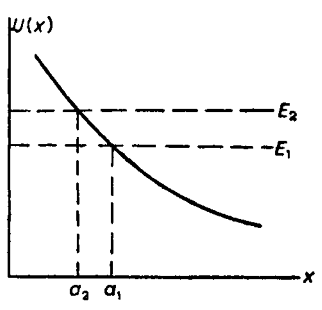

FIG. 17

According to (47.5), the wave function ψ_1 in the regions on both sides of the turning-point $x = a_1$, but not in its immediate neighbourhood, is of the form

$$\left.\begin{aligned} \text{for } x < a_1, \quad \psi_1 &= \frac{C_1}{2\sqrt{|p_1|}} \exp\left[-\frac{1}{\hbar}\int_{a_1}^{x} p_1\,\mathrm{d}x\right], \\ \text{for } x > a_1, \quad \psi_1 &= \frac{C_1}{\sqrt{p_1}} \cos\left(\frac{1}{\hbar}\int_{a_1}^{x} p_1\,\mathrm{d}x - \tfrac{1}{4}\pi\right), \end{aligned}\right\} \tag{51.2}$$

and similarly for ψ_2 (replacing the suffix 1 by 2).

However, the calculation of the integral (51.1) by substituting in it these asymptotic expressions for the wave functions would not give the correct result. The reason is, as we shall see below, that this integral is an exponentially small quantity, whereas the integrand is not itself small. Hence even a relatively small change in the integrand will in general change the order of magnitude of the integral. This difficulty can be circumvented as follows.

We represent the function ψ_2 as a sum $\psi_2 = \psi_2^+ + \psi_2^-$, expressing the cosine (in the region $x > a_2$) as the sum of two exponentials. According to (50.2), we have

$$\left.\begin{aligned} \text{for } x < a_2, \quad \psi_2^+ &= \frac{C_2}{2\sqrt{|p_2|}} \exp\left[\frac{1}{\hbar}\left|\int_{a_2}^{x} p_2\,\mathrm{d}x\right|\right], \\ \text{for } x > a_2, \quad \psi_2^+ &= \frac{C_2}{2\sqrt{p_2}} \exp\left[\frac{i}{\hbar}\int_{a_2}^{x} p_2\,\mathrm{d}x + \tfrac{1}{4}i\pi\right]; \end{aligned}\right\} \tag{51.3}$$

the function ψ_2^- is the complex conjugate of $\psi_2^+ : \psi_2^- = (\psi_2^+)^*$.

The integral (51.1) is also divided into the sum of two complex conjugate integrals $f_{12} = f_{12}^+ + f_{12}^-$, which we shall proceed to calculate. First of all, we note that the integral

$$f_{12}^+ = \int_{-\infty}^{\infty} \psi_1 f \psi_2^+\,\mathrm{d}x$$

converges. For, although the function ψ_2^+ increases exponentially in the region $x < a_2$, the function ψ_1, in the region $x < a_1$, tends exponentially to zero still more rapidly (since we have $|p_1| > |p_2|$ everywhere in the region $x < a_2$).

We shall regard the coordinate x as a complex variable, and displace the path of integration off the real axis into the upper half-plane. When x receives a positive imaginary increment, an increasing term appears in the function ψ_1 (in the region $x > a_1$), but the function ψ_2^+ decreases still more rapidly, since we have $p_2 > p_1$ everywhere in the region $x > a_1$. Hence the integrand decreases.

The displaced path of integration does not pass through the points $x = a_1$, a_2 on the real axis, near which the quasi-classical approximation is inapplicable. Hence we can use for ψ_1 and ψ_2^+, over the whole path, the functions which are their asymptotic expressions in the upper half-plane. These are

$$\left.\begin{aligned} \psi_1 &= \frac{C_1}{2[2m(U-E_1)]^{1/4}} \exp\left[\frac{1}{\hbar}\int_{a_1}^{x} \sqrt{\{2m(U-E_1)\}}\,\mathrm{d}x\right], \\ \psi_2^+ &= \frac{C_2}{2[2m(U-E_2)]^{1/4}} \exp\left[-\frac{1}{\hbar}\int_{a_2}^{x} \sqrt{\{2m(U-E_2)\}}\,\mathrm{d}x\right], \end{aligned}\right\} \tag{51.4}$$

where the roots are taken so as to be positive on the real axis for $x < a_1, a_2$.

In the integral

$$f_{12}^+ = \frac{C_1C_2}{4\sqrt{(2m)}} \int \exp\left[\frac{1}{\hbar}\int_{a_1}^{x} \sqrt{\{2m(U-E_1)\}}\,\mathrm{d}x - \frac{1}{\hbar}\int_{a_2}^{x} \sqrt{\{2m(U-E_2)\}}\,\mathrm{d}x\right] \times \\ \times \frac{f(x)\,\mathrm{d}x}{[(U-E_1)(U-E_2)]^{1/4}} \tag{51.5}$$

we desire to displace the path of integration in such a way that the exponential factor is diminished as much as possible. The exponent has an extreme value only where $U(x) = \infty$ (for $E_1 \neq E_2$, its derivative with respect to x vanishes at no other point). Hence the displacement of the contour of integration into the upper half-plane is restricted only by the necessity of passing round the singular points of the function $U(x)$; according to the general theory of linear differential equations, these coincide with the singular points of the wave function $\psi(x)$. The actual choice of the contour depends on the actual form of the field $U(x)$. Thus, if the function $U(x)$ has only one singular point $x = x_0$ in the upper half-plane, the integration can be effected along the type of path shown in Fig. 18. The immediate neighbourhood of the singular point plays the important part in the integral, so that the matrix element $f_{12} = 2\,\mathrm{re}\,f_{12}^+$ required is practically proportional to an exponentially small expression of the form

$$f_{12} \sim \exp\left\{-\frac{1}{\hbar}\mathrm{im}\left[\int^{x_0} \sqrt{[2m(E_2-U)]}\,\mathrm{d}x - \int^{x_0} \sqrt{[2m(E_1-U)]}\,\mathrm{d}x\right]\right\} \tag{51.6}$$

(L. D. Landau 1932).†

† In deriving formulae (51.5) and (51.6), we have replaced the wave functions by their asymptotic expressions, since, in the integral taken along the contour shown in Fig. 18 (p. 188), the order of magnitude of the integral is determined by that of the integrand; hence a relatively small change in the latter does not have any great effect on the value of the integral.

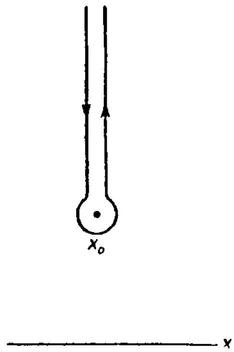

FIG. 18

The lower limits of the integrals may be any points in the classically accessible regions; their particular values evidently do not affect the imaginary parts of the integrals. If the function $U(x)$ has several singular points in the upper half-plane, x_0 in (51.6) must be taken as that for which the exponent is smallest in absolute value.†

The quasi-classical matrix elements for motion in a centrally symmetric field must be calculated by the same method. However, we must now replace $U(r)$ by the effective potential energy (the sum of the potential energy and the centrifugal energy), which will be different for states with different l. In view of further applications of the method in question, we shall write the effective potential energies in the two states in a general form, as $U_1(r)$ and $U_2(r)$. Then the exponent in the exponential factor in the integrand in (51.5) has an extreme value not only at the points where $U_1(r)$ or $U_2(r)$ becomes infinite, but also at those where

$$U_2(r)-U_1(r) = E_2-E_1. \tag{51.7}$$

Hence, in the formula

$$f_{12} \sim \exp\left\{-\frac{1}{\hbar}\,\mathrm{im}\left[\int^{r_0}\sqrt{[2m(E_2-U_2)]}\,\mathrm{d}r-\int^{r_0}\sqrt{[2m(E_1-U_1)]}\,\mathrm{d}r\right]\right\} \tag{51.8}$$

the possible values of r_0 include not only the singular points of $U_1(r)$ and $U_2(r)$, but also the roots of equation (51.7).

The centrally symmetric case differs also in that the integration over r in (51.1) is taken from 0 (and not from $-\infty$) to ∞:

$$f_{12} = \int_0^\infty \chi_1 f \chi_2\,\mathrm{d}r.$$

Here two cases must be distinguished. If the integrand is an even function of r, the integration can be formally extended to the whole range from $-\infty$

† We assume that the quantity $f(x)$ itself has no singular points.

to ∞, so that there is no difference from the previous case. This may occur if $U_1(r)$ and $U_2(r)$ are even functions of r $[U(-r) = U(r)]$. Then the wave functions $\chi_1(r)$ and $\chi_2(r)$ are either even or odd functions† (see §21), and, if the function $f(r)$ is also even or odd, the product $\chi_1 f \chi_2$ may be even.

If, on the other hand, the integrand is not even (as always happens if $U(r)$ is not even), the start of the path of integration cannot be moved away from the point $r = 0$, and this point must be included among the possible values of r_0 in (51.8).

PROBLEMS

PROBLEM 1. Calculate the quasi-classical matrix elements (exponential factor only) in a field $U = U_0 e^{-\alpha x}$.

SOLUTION. $U(x)$ becomes infinite only for $x \to -\infty$. Accordingly, we put $x_0 = -\infty$ in (51.6). We can extend the integration to $+\infty$.

Each of the integrals diverges at the lower limit. Hence we first calculate them from $-x$ to ∞, and then pass to the limit $x \to \infty$. We find

$$f_{12} \sim e^{-(\pi m/\alpha\hbar)(v_2 - v_1)},$$

where $v_1 = \sqrt{(2E_1/m)}$, $v_2 = \sqrt{(2E_2/m)}$ are the velocities of the particle at infinity ($x \to \infty$), where the motion is free.

PROBLEM 2. The same as Problem 1, but in a Coulomb field $U = \alpha/r$, for transitions between states with $l = 0$.

SOLUTION. The only singular point of the function $U(r)$ is $r = 0$. The corresponding integral has been calculated in §50, Problem 2. As a result we have by formula (51.8)

$$f_{12} \sim \exp\left[\frac{\pi\alpha}{\hbar}\left(\frac{1}{v_2} - \frac{1}{v_1}\right)\right].$$

§52. The transition probability in the quasi-classical case

Penetration through a potential barrier is an example of a process which is entirely impossible in classical mechanics. In the quasi-classical case the probability of such processes is exponentially small. The relevant exponent can be determined as follows.

Considering a transition of any system from one state to another, we solve the corresponding classical equations of motion and find the "path" of the transition; this, however, is complex, in accordance with the fact that the process cannot occur in classical mechanics. In particular, it is found that, in general, the "transition point" q_0 at which the formal transition of the system from one state to the other occurs is complex; the position of this point is determined by the classical conservation laws. We next calculate the action $S_1(q_1, q_0) + S_2(q_0, q_2)$ for the motion of the system in the first state from some initial position q_1 to the "transition point" q_0, and then in the second state from q_0 to the final position q_2. The required probability of the process is then given by the formula

$$w \sim \exp\left\{-\frac{2}{\hbar}\,\mathrm{im}\,[S_1(q_1,q_0) + S_2(q_0,q_2)]\right\}. \tag{52.1}$$

† For even $U(r)$, the radial wave function $R(r)$ is even (or odd) when l is even (or odd), as is seen from its behaviour for small r (where $R \sim r^l$).

If the position of the "transition point" is not unique, it must be chosen so that the exponent in (52.1) has the smallest absolute value (which must yet, of course, be sufficiently large for formula (52.1) to be valid).†

Formula (52.1) is in accordance with the rule derived in §51 for calculating the quasi-classical matrix elements. It should be emphasized, however, that it would not be correct to use the square of the matrix element in calculating the coefficient before the exponential in the probability of such transitions.

The method of *complex classical paths* based on (52.1) is a general one, applicable to transitions in systems with any number of degrees of freedom (L. D. Landau 1932). If the transition point is real, but lies in the classically inaccessible region, then (in the simple case of one-dimensional motion) formula (52.1) is the same as (50.5) for the probability of penetration through the potential barrier.

Reflection above the barrier

Let us apply (52.1) to the one-dimensional problem of reflection above the barrier, i.e. reflection of a particle whose energy exceeds the height of the barrier. In this case, q_0 is to be taken as the complex coordinate x_0 of the "turning point" at which the particle reverses its direction of motion, i.e. the complex root of the equation $U(x) = E$. We shall show how the reflection coefficient may then be calculated more precisely, including the coefficient of the exponential.

We must again (as in §50) establish the relation between the wave functions far to the right of the barrier (the transmitted wave) and far to the left (the incident and reflected waves). This is easily done by a method similar to that used in §§47 and 50, regarding ψ as a function of the complex variable x.

We write the transmitted wave in the form

$$\psi_+ = \frac{1}{\sqrt{p}} \exp\left(\frac{i}{\hbar}\int_{x_1}^{x} p \, dx\right),$$

where x_1 is any point on the real axis, and follow its variation on passing along a path C in the upper half-plane which encloses (at a sufficient distance) the turning point x_0 (Fig. 19); the whole of the latter part of this path must lie so far to the left that the error in the approximate (quasi-classical) wave function of the incident wave is less than the required small quantity ψ_-. Passage round the point x_0 causes a change in the sign of the root $\sqrt{[E-U(x)]}$, and after the return to the real axis the function ψ_+ therefore becomes ψ_-, a wave propagated to the left (i.e. the reflected wave).‡ Since the amplitudes of the incident and transmitted waves may be regarded as equal, the

† If the potential energy of the system has itself singular points, these also must be considered as possible values of q_0.

‡ A passage along a path below the point x_0 (simply going along the real axis, for example) converts the function ψ_+ into the incident wave.

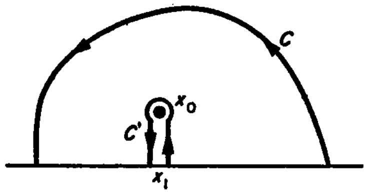

FIG. 19

required reflection coefficient R is simply the ratio of the squared moduli of ψ_- and ψ_+:

$$R = \left|\frac{\psi_-}{\psi_+}\right|^2 = \exp\left(-\frac{2}{\hbar}\,\mathrm{im}\int_C p\,\mathrm{d}x\right). \tag{52.2}$$

Having derived this formula, we can deform the path of integration in the exponent in any manner; if we convert it into the path C' shown in Fig. 19, the integral reduces to twice the integral from x_1 to x_0, giving

$$R = \exp\left(-4\sigma(x_1, x_0)/\hbar\right), \quad \sigma(x_1, x_0) = \mathrm{im}\int_{x_1}^{x_0} p(x)\,\mathrm{d}x; \tag{52.3}$$

since $p(x)$ is real everywhere on the real axis, the choice of x_1 is immaterial. Note that the coefficient of the exponential in (52.3) is unity (V. L. Pokrovskii, S. K. Savvinykh and F. R. Ulinich 1958).†

As already mentioned, among the possible values of x_0 we must select the one for which the exponent in (52.3) is smallest in absolute magnitude (and this value must be large compared with unity).‡ It is also implied that, if the potential energy $U(x)$ itself has singularities in the upper half-plane, the integral $\sigma(x_1, x_0)$ has larger values for such points; otherwise the exponent would be determined by one of these points, but the coefficient of the exponential would not be unity as in (52.3). This condition is certainly not satisfied with increasing energy E if $U(x)$ becomes infinite anywhere in the upper half-plane: ultimately the point x_0 at which $U = E$ becomes so close to the point x_∞ where $U = \infty$ that the two points give comparable contributions to the reflection coefficient (the integral $\sigma(x_\infty, x_0) \sim 1$), and formula (52.3) becomes invalid. In the limit where E is so large that this integral is small compared with unity, perturbation theory becomes applicable (see Problem 2).‖

† The proof given here is due to L. D. Landau (1961).

‡ Of course, only points x_0 are considered for which $\sigma > 0$, i.e. points lying in the upper half-plane.

‖ An intermediate case is discussed by V. L. Pokrovskii and I. M. Khalatnikov, *Soviet Physics JETP* **13**, 1207, 1961.

PROBLEMS

PROBLEM 1. Using the quasi-classical approximation, with exponential accuracy, determine the probability of disintegration of a deuteron in collision with a heavy nucleus regarded as the fixed centre of a Coulomb field (E. M. Lifshitz 1939).

SOLUTION. The principal contribution to the reaction probability comes from collisions with zero orbital angular momentum. In the quasi-classical approximation these are the head-on collisions, in which the movement of the particles becomes one-dimensional.

Let E be the deuteron energy in units of ϵ, the binding energy of the proton and the neutron in the deuteron; E_n and E_p the energies of the released neutron and proton in the same units. We shall also use the dimensionless coordinate $q = \epsilon r/Ze^2$ (where Ze is the charge on the nucleus), and denote by q_0 its value (which is in general complex) at the "transition point", i.e. at the "moment of disintegration" of the deuteron. We can write

$$E_n = \tfrac{1}{2}v_n^2, \qquad E_p = \tfrac{1}{2}v_p^2 + \frac{1}{q_0}, \qquad E = v_d^2 + \frac{1}{q_0}; \tag{1}$$

here v_n, v_p and v_d are the velocities of the particles at the moment of disintegration, in units of $\sqrt{(\epsilon/m)}$, where m is the nucleon mass; v_n is real and is the same as the velocity of the released neutron, but v_p and v_d are complex. The conditions for the conservation of energy and momentum at the transition point give

$$E_p + E_n = E - 1, \qquad v_p + v_n = 2v_d, \tag{2}$$

whence

$$v_p = 2i + v_n, \qquad v_d = i + v_n, \qquad \frac{1}{q_0} = E + 1 - v_n^2 + 2iv_n.$$

The action of the system before the transition corresponds to the motion of the deuteron in the field of the nucleus up to the point of disintegration; its imaginary part is

$$\begin{aligned} \operatorname{im} S_1 &= Ze^2\sqrt{\frac{m}{\epsilon}}\operatorname{im}\int_{\infty}^{q_0}\sqrt{\left[4\left(E-\frac{1}{q}\right)\right]}\,\mathrm{d}q \\ &= Ze^2\sqrt{\frac{m}{\epsilon}}\operatorname{im}\left\{2q_0v_d - \frac{2}{\sqrt{E}}\cosh^{-1}\sqrt{(q_0E)}\right\}. \end{aligned} \tag{3}$$

After the transition, the action corresponds to the motion of the neutron and the proton away from the point of disintegration:

$$\begin{aligned} \operatorname{im} S_2 &= Ze^2\sqrt{\frac{m}{\epsilon}}\operatorname{im}\left\{\int_{q_0}^{\infty} v_n\,\mathrm{d}q + \int_{q_0}^{\infty}\sqrt{\left[2\left(E_p - \frac{1}{q}\right)\right]}\,\mathrm{d}q\right\} \\ &= Ze^2\sqrt{\frac{m}{\epsilon}}\operatorname{im}\left\{-v_nq_0 - v_pq_0 + \sqrt{\frac{2}{E_p}}\cosh^{-1}\sqrt{(q_0E_p)}\right\}. \end{aligned} \tag{4}$$

According to (52.1), the probability of the process is

$$w \sim \exp\left\{-\frac{2Ze^2}{\hbar}\sqrt{\frac{m}{\epsilon}}\operatorname{im}\left[\sqrt{\frac{2}{E_p}}\cosh^{-1}\sqrt{(q_0E_p)} - \frac{2}{\sqrt{E}}\cosh^{-1}\sqrt{(q_0E)}\right]\right\}. \tag{5}$$

In accordance with the fact that the two inverse hyperbolic cosines here come from (4) and (3), the signs of their imaginary parts must be the same as those of im v_p and im v_d respectively, and the signs of the latter in the solution of equations (2) are chosen so as to make $\operatorname{im}(S_1+S_2) > 0$.

Because w depends exponentially on E_n, the total probability of disintegration (with any values of E_n and $E_p = E-1-E_n$) is given by the minimum absolute value of the exponent as a function of E_n. Analysis shows that this occurs when $E_n \to 0$. Then $q_0 = 1/(E+1)$, and from (5) we find

$$w \sim \exp\left\{-\frac{2Ze^2}{\hbar}\sqrt{\frac{m}{\epsilon}}\left[\sqrt{\frac{2}{E-1}}\cos^{-1}\sqrt{\frac{E-1}{E+1}}-\frac{2}{\sqrt{E}}\cos^{-1}\sqrt{\frac{E}{E+1}}\right]\right\}.$$

The condition for this formula to be valid is that the exponent should be large compared with unity.

Having calculated the imaginary part of the action $S = S_1+S_2$ for non-zero values of E_n, we can find the energy distribution of the particles released. Near $E_n = 0$, we have†

$$\operatorname{im} S(E_n) - \operatorname{im} S(0) \approx E_n\left[\frac{d \operatorname{im} S}{dE_n}\right]E_n = 0.$$

A calculation of the derivative gives

$$\frac{dw}{dE_n} \sim \exp\left\{-\frac{2Ze^2}{\hbar}\sqrt{\frac{m}{\epsilon}}E_n\left[\frac{3-E}{(E-1)(E+1)^2}+\frac{1}{\sqrt{[2(E-1)^3]}}\cos^{-1}\sqrt{\frac{E-1}{E+1}}\right]\right\}.$$

PROBLEM 2. Determine the coefficient of reflection above the barrier for particle energies such that perturbation theory is applicable.

SOLUTION. Formula (43.1) is used, the initial and final wave functions being plane waves propagated in opposite directions and normalized respectively by unit current density and the delta function of momentum divided by $2\pi\hbar$, with $d\nu = dp'/2\pi\hbar$ and p' the momentum after reflection. Carrying out the integration with respect to p' (taking account of the delta function), we obtain

$$R = \frac{m^2}{\hbar^2 p^2}\left|\int_{-\infty}^{\infty} U(x)e^{2ipx/\hbar}\,dx\right|^2. \tag{1}$$

This formula is valid if the conditions for perturbation theory to be applicable are satisfied: $Ua/\hbar v \ll 1$, where a is the width of the barrier (see the third footnote to §45), and also $pa/\hbar \lesssim 1$. The latter condition ensures that the function $R(p)$ is not exponential; otherwise the question of the validity of formula (1) would require further investigation.

PROBLEM 3. Determine the coefficient of reflection above the barrier for a quasi-classical barrier when the function $U(x)$ has a discontinuity of slope at $x = x_0$.

SOLUTION. If the function $U(x)$ has a singularity for real x, the reflection coefficient is determined mainly by the field near that point, and perturbation theory can be formally applied to calculate it, without having to be valid for all x; the fulfilment of the quasi-classical condition is sufficient. We then have formula (1) of Problem 2, the only difference being that the momentum of the incident particle must be replaced by the value of $p(x)$ at the singular point.

In this case we take the point of discontinuous slope as $x = 0$, and thus have near this point

$$U = -F_1 x \quad \text{for} \quad x > 0, \qquad U = -F_2 x \quad \text{for} \quad x < 0,$$

with different F_1 and F_2. The integration with respect to x is effected by including in the integrand a damping factor $e^{\pm\lambda x}$ and then letting $\lambda \to 0$. The result is

$$R = \frac{m^2\hbar^2}{16p_0^6}(F_2-F_1)^2,$$

where $p_0 = p(0)$.

† When $E_n = 0$, the function $\operatorname{im} S(E_n)$ has a cusp from which it increases for both positive and negative E_n (the negative values corresponding to the capture of the neutron by the nucleus).

§53. Transitions under the action of adiabatic perturbations

It has already been mentioned in §41 that, in the limit of a perturbation which varies arbitrarily slowly with time, the probability of a transition of a system from one state to another tends to zero. Let us now consider this problem quantitatively, by calculating the transition probability under the action of a slowly varying (adiabatic) perturbation (L. D. Landau 1961).

Let the Hamiltonian of the system be a slowly varying function of time, tending to definite limits as $t \to \pm\infty$, and let $\psi_n(q, t)$ and $E_n(t)$ be the eigenfunctions and the eigenvalues of the energy (depending on time as a parameter) obtained by solving Schrödinger's equation $\hat{H}(t)\psi_n = E_n\psi_n$; on account of the adiabatic variation of $\hat{H}$ with time, the time variation of E_n and ψ_n with time will also be slow. The problem is to determine the probability w_{21} of finding the system in a certain state ψ_2 as $t \to +\infty$, if it was in the state ψ_1 as $t \to -\infty$.

The slow variation of the perturbation means that the duration of the "transition process" is very long, and therefore the change in the action during this time (given by the integral $-\int E(t)\,\mathrm{d}t$) is large. In this sense the problem is quasi-classical, and the required probability is mainly determined by the values t_0 of t for which

$$E_1(t_0) = E_2(t_0) \tag{53.1}$$

and which correspond, as it were, to the "instant of transition" in classical mechanics (cf. §52); in reality, of course, such a transition is classically impossible, as is shown by the fact that the roots of equation (53.1) are complex. It is therefore necessary to examine the properties of the solutions of Schrödinger's equation for complex values of the parameter t in the neighbourhood of the point $t = t_0$ at which the two eigenvalues of the energy become equal.

As we shall see, the eigenfunctions ψ_1, ψ_2 vary rapidly with t near this point. To determine this dependence, we first define linear combinations ϕ_1, ϕ_2 of ψ_1, ψ_2 which satisfy the conditions

$$\int \phi_1^2\,\mathrm{d}q = \int \phi_2^2\,\mathrm{d}q = 0, \qquad \int \phi_1\phi_2\,\mathrm{d}q = 1. \tag{53.2}$$

This can always be achieved by suitable choice of the complex coefficients (which are functions of t). The functions ϕ_1, ϕ_2 have no singularity at $t = t_0$.

We now seek the eigenfunctions as linear combinations

$$\psi = a_1\phi_1 + a_2\phi_2. \tag{53.3}$$

Here it must be borne in mind that, when the "time" t is complex, the operator $\hat{H}(t)$ (of the form (17.4)) is still equal to its transpose ($\hat{H} = \tilde{\hat{H}}$), but is no longer Hermitian ($\hat{H} \neq \tilde{\hat{H}}^*$), since the potential energy $U(t) \neq U^*(t)$.

We substitute (53.3) in Schrödinger's equation, multiply on the left by

ϕ_1 or ϕ_2, and integrate with respect to q. With the notation

$$H_{ik}(t) = \int \phi_i \hat{H} \phi_k \, dq, \tag{53.4}$$

and using the fact that $H_{12} = H_{21}$ owing to the above-mentioned property of the Hamiltonian, we obtain the equations

$$\left.\begin{aligned} H_{11}a_1 + H_{12}a_2 &= Ea_2, \\ H_{12}a_1 + H_{22}a_2 &= Ea_1. \end{aligned}\right\} \tag{53.5}$$

The condition for these equations to have non-zero solutions is $(H_{12}-E)^2 = H_{11}H_{22}$, and the roots of this give the energy eigenvalues

$$E = H_{12} \pm \sqrt{(H_{11}H_{22})}. \tag{53.6}$$

Then (53.5) gives

$$a_2/a_1 = \pm\sqrt{(H_{11}/H_{22})}. \tag{53.7}$$

It is seen from (53.6) that, for a coincidence at the point $t = t_0$ of the two eigenvalues, either H_{11} or H_{22} must vanish at that point; let H_{11} vanish there. At a regular point, a function in general vanishes as $t-t_0$, and therefore

$$E(t) - E(t_0) = \pm \text{constant} \times \sqrt{(t-t_0)}, \tag{53.8}$$

i.e. $E(t)$ has a branch point at $t = t_0$. We also have $a_2 \sim \sqrt{(t-t_0)}$, and so there is at the point $t = t_0$ only one eigenfunction, ϕ_1.

We now see that the problem is formally completely analogous to the problem of reflection above the barrier discussed in §52. We have a wave function $\Psi(t)$ which is "quasi-classical with respect to time", instead of the function quasi-classical with respect to the coordinate in §52, and wish to find the term of the form $c_2\psi_2 e^{-iE_2t/\hbar}$ in the wave function for $t \to +\infty$, if the wave function $\Psi(t) = \psi_1 e^{-iE_1t/\hbar}$ as $t \to -\infty$. This is analogous to the problem of determining the reflected wave for $x \to -\infty$ from the transmitted wave for $x \to +\infty$. The required transition probability $w_{21} = |c_2|^2$. The action $S = -\int E(t)\,dt$ is given by the time integral of a function having complex branch points (just as the function $p(x)$ in the integral $\int p\,dx$ had complex branch points). The problem under consideration is therefore dealt with by means of a contour in the plane of the complex variable t from large negative to large positive values, just as in §52 for the plane of the variable x, and we shall not repeat the derivation here.

We shall suppose that $E_2 > E_1$ on the real axis. Then the contour must lie in the upper half-plane of the complex variable t (where the ratio $e^{-iE_2t/\hbar}/e^{-iE_1t/\hbar}$ increases). The resulting formula (analogous to (52.2)) is

$$w_{21} = \exp\left(\frac{2}{\hbar}\,\mathrm{im}\int_{C'} E(t)\,dt\right), \tag{53.9}$$

where the integration is along the contour shown in Fig. 19 (from left to right).

On the left-hand branch of this contour $E = E_1$, and on the right-hand branch $E = E_2$. We can therefore write (53.9) in the form

$$w_{21} = \exp\left(-2\,\mathrm{im}\int_{t_1}^{t_0} \omega_{21}(t)\,\mathrm{d}t\right), \qquad (53.10)$$

where $\omega_{21} = (E_2 - E_1)/\hbar$, and t_1 is any point on the real axis of t; t_0 must be taken as that root of equation (53.1) lying in the upper half-plane for which the exponent in (53.10) is smallest in absolute value.† In addition, besides the direct transition from state 1 to state 2, there may be possible paths through various intermediate states; the probabilities of these are given by analogous formulae. For example, for a transition $1 \to 3 \to 2$ the integral in (53.10) is replaced by a sum of integrals:

$$\int^{t_0^{(31)}} \omega_{31}(t)\,\mathrm{d}t + \int^{t_0^{(23)}} \omega_{23}(t)\,\mathrm{d}t,$$

where the upper limits are the "points of intersection" of the terms $E_1(t)$, $E_3(t)$ and $E_3(t)$, $E_2(t)$ respectively. This result is obtained by means of a contour which encloses both these complex points.‡

† The possible values of t_0 must include any points at which $E(t)$ becomes infinite; for such points the coefficient of the exponential in (53.9) will not be unity.

‡ The intermediate states of a continuous spectrum require a special discussion.