THE WKB METHOD FOR A COMPLEX POTENTIAL

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Summary

The extension of the WKB method to a complex potential, as used in the optical model of the nucleus, is discussed. The formula for the complex phase shifts is formally deduced, and its accuracy tested against exact calculations for a square potential well and a well with sloping sides. At low energies there occur large discrepancies; the WKB phases vary regularly with energy, whereas the exact values oscillate violently about the WKB values in a characteristic way and marked resonances occur. The factors affecting the accuracy of the method are discussed.

At higher energies the fluctuation of the phases about the WKB value is less marked, and its effect largely cancels out as the result of a larger number of phases being involved in the scattering.

I. Introduction

The WKB method for the determination of phase shifts in collision problems has been remarkably useful, notably in the scattering of electrons by atoms (Massey and Burhop 1952), and its range of validity is well understood. With the success of the optical model of the nucleus, in which a potential with an imaginary component is used, there arises the question of the correct method of application of the WKB method to a complex potential and its range of validity.

The method has been found valid for nucleons incident on nuclei with energies large compared with the nuclear potential (Mohr and Robson 1956), in which case one may use an obvious approximation to the WKB formula (Massey and Mohr 1934). In this approximation the ratio of the imaginary to the real component of the phase is equal to the ratio of the imaginary to the real component of the well depth.

At lower energies, in a calculation of α-particle scattering with a comparatively large imaginary well depth, B. A. Robson (unpublished data) in this laboratory recently found that a tentative adaption of the WKB formula without approximation gave an imaginary component of the phase many times the value given by numerical integration of the wave equation.

An examination of the situation seemed to be called for, including a formal justification of the natural generalization of the WKB method for a complex potential, in order to see whether extra approximations were involved.

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II. Deduction of the Formula

For a potential $V=V_r+\mathrm{i}V_i$, the modified radial equation for the lth order wave is

$$u''+(U+\mathrm{i}W)u=0,$$

where

$$U=2m\hbar^{-2}(E+V_r)-l(l+1)r^{-2},\quad W=2m\hbar^{-2}V_i,$$

primes here and later denoting differentiation with respect to r. The solution will be of the form

$$u=F\sin\varphi+\mathrm{i}G\cos\chi,$$

where F, G, φ, and χ are functions of r. To avoid unduly complicated formulae we make the approximation $\chi=\varphi$, which we shall find is a good approximation for a constant V, i.e. for the greater part of a nucleus. Substituting this form for u in the differential equation, and equating separately to zero the coefficients of $\sin\varphi$ and $\cos\varphi$ in both the real and imaginary terms, we obtain

$$F''-F\varphi'^2=-UF, \quad \ldots\ldots\ldots\ldots \quad (1a)$$

$$F\varphi''+2F'\varphi'=WG, \quad \ldots\ldots\ldots\ldots \quad (1b)$$

and similar equations with F and G interchanged. Putting

$$F=C\cosh\xi,\quad G=C\sinh\xi \quad \ldots\ldots\ldots\ldots \quad (2)$$

gives, on neglecting terms of second order,

$$\varphi'^2-\xi'^2=U,$$
$$2\varphi'\xi'=W.$$

If we write $(U+\mathrm{i}W)^{\frac{1}{2}}=P+\mathrm{i}Q$, where the principal values of P and Q are taken, then we have

$$\varphi=\int^r P\mathrm{d}r,\quad \xi=\int^r Q\mathrm{d}r. \quad \ldots\ldots\ldots\ldots \quad (3)$$

From (3) we have

$$\varphi'=P. \quad \ldots\ldots\ldots\ldots \quad (4)$$

From (1b) we obtain $\mathrm{d}(F^2\varphi')/\mathrm{d}r=WFG$. Subtracting the corresponding equation with F and G interchanged, integrating the result, and using (4) gives

$$F^2-G^2=A^2P^{-1},$$

where A^2 is the constant of integration. Substituting (2) then gives

$$C=AP^{-\frac{1}{2}}.$$

The radial equation therefore has the solution

$$u=AP^{-\frac{1}{2}}\sin(\varphi+\mathrm{i}\xi) \quad \ldots\ldots\ldots\ldots \quad (5)$$

with φ and ξ given by (3). A is fixed by normalizing the wave function. The formula (5) would result from the obvious generalization of the WKB method

to a complex potential; but our deduction shows that in addition to the approximations inherent in the ordinary WKB method, the further approximation $\chi=\varphi$ is involved. We shall find that this approximation is good only for a constant potential.

In the absence of a scattering potential

$$u=A_0U_0^{-\frac{1}{4}}\sin(\varphi_0+\mathrm{i}\xi_0),$$

where the suffix nought denotes values obtained with $V_r=0=V_i$. The lth order phase η is therefore given to a first approximation by

$$\eta=(\varphi-\varphi_0)+\mathrm{i}(\xi-\xi_0). \quad \ldots\ldots\ldots\ldots \quad (6)$$

On analogy with the Langer modification of the WKB method for real potentials, one might expect (6) to give improved values on taking $(l+\frac{1}{2})^2$ in place of $l(l+1)$ in each integrand.

The question of the lower limits of integration in (3) has now to be settled, for none of the integrands has a zero as for real V. Examination of the behaviour of the integrands in specific cases indicates that with little error one may take the lower limit of integration to be zero. For as r decreases below the classical distance of closest approach, ξ and ξ_0 both become large but their difference diminishes rapidly. We shall now test these conclusions for the case of a constant potential.

III. Improvement and Test of the Formula for a Constant Potential

The WKB method for a real potential $V=V_r$ gives

$$u=U^{-\frac{1}{4}}\sin\theta, \quad \text{where } \theta=\tfrac{1}{4}\pi+\int_{r_0}^{r}U^{\frac{1}{2}}\mathrm{d}r, \quad \ldots\ldots\ldots \quad (7)$$

and r_0 is the zero of U. It may easily be shown that, for constant V_r, this value of u reduces to r times the Debye asymptotic expansion of the spherical Bessel function $\mathrm{j}_l(K_rr)$ where $K_r^2=2m\hbar^{-2}(E+V_r)$. One finds that the Debye form, which is much more accurate than the ordinary form of the asymptotic expansion, gives the first zero of $\mathrm{j}_l(x)$ to an accuracy of about $0\cdot05$ in x, and higher zeros with smaller errors, up to quite high orders l. (7) will therefore be accurate for real and constant V.

For complex $z=x+\mathrm{i}y$, the values of x which make $\mathrm{Re}\,\mathrm{j}_l(z)$ zero are still given better, though not nearly so much better, by the Debye form than by the ordinary form of the asymptotic expansion of $\mathrm{j}_l(z)$; but the values are found to be given best of all by the zeros of $\mathrm{j}_l(x)$. This result may be seen as follows. From Taylor's theorem

$$\mathrm{Re}\,u(x+\mathrm{i}y)=u(x)-\tfrac{1}{2}y^2u''(x)+\ldots$$

At a zero of $u(x)$ we have $u=0$, and hence, from the form of the differential equation for u, $u''(x)$ and higher even derivatives will be small, provided U is slowly varying and W is small. Under these conditions, then, the zeros of

Re $u(x+iy)$ will be relatively independent of y for small y. A better approximation to η than (6) will therefore be

$$\eta=(\theta-\theta_0)+i(\xi-\xi_0). \quad \ldots\ldots\ldots\ldots\ldots \quad (8)$$

To test the accuracy of phases calculated from (8), comparison was made with phases calculated exactly for a square well in the usual way (Mott and Massey 1949) with complex values taken for the wave numbers. The test was made particularly stringent by the choice of a low incident energy, for which the WKB method would not be expected to be so accurate, namely, 4 MeV neutrons. Taking a nucleus of mass number 100 and a well depth of $42+4\cdot6i$ MeV, we obtain $kR=3$, $KR=10+0\cdot5i$, where K and k are 2π times the interior and exterior wave numbers respectively, and R is the nuclear radius. The exact values obtained for the various order phases are given in Table 1, in the second column. The real part was found to be well within 1 per cent., in nearly every case, of the value of the corresponding phases for $KR=10$, justifying preference for (8) rather than (6).

TABLE 1

PHASES OF ORDER l FOR 4 MeV NEUTRONS INCIDENT ON A NUCLEUS OF MASS NUMBER 100, REPRESENTED BY A SQUARE WELL OF DEPTH $(42+4\cdot6i)$ MeV, FOR WHICH $kR=3$, $KR=10+0\cdot5i$

l	Exact Method	WKB Method		Born Approximation
		Formula (8)	Formula (9)	
0	$6\cdot58+0\cdot17i$	$6\cdot97+0\cdot50i$	$6\cdot60+0\cdot17i$	$15\cdot87+1\cdot75i$
1	$7\cdot47+0\cdot25i$	$6\cdot73+0\cdot49i$	$7\cdot48+0\cdot24i$	$14\cdot39+1\cdot59i$
2	$5\cdot61+0\cdot16i$	$6\cdot19+0\cdot48i$	$5\cdot62+0\cdot16i$	$5\cdot00+0\cdot55i$
3	$5\cdot96+0\cdot07i$	$5\cdot12+0\cdot46i$	$5\cdot96+0\cdot07i$	$0\cdot87+0\cdot96i$
4	$3\cdot13+0\cdot08i$	$3\cdot96+0\cdot44i$	$3\cdot13+0\cdot08i$	$0\cdot09+0\cdot01i$
5	$3\cdot14+0\cdot002i$	$2\cdot86+0\cdot41i$	$3\cdot14+0\cdot002i$	$0\cdot01+0\cdot001i$
6	$3\cdot14+0\cdot000i$	$1\cdot99+0\cdot37i$	$3\cdot14+0\cdot000i$	$0\cdot00+0\cdot000i$
7	$0\cdot00+0\cdot000i$	$1\cdot19+0\cdot32i$	$0\cdot00+0\cdot000i$	
8		$0\cdot55+0\cdot25i$		
9		$0\cdot11+0\cdot15i$		

The WKB phases given by (8) with the Langer modification are shown in the third column of the table. Large errors are evident, which may be classified into three types: (i) the real component varies regularly with l, whereas the real component of the exact phases jumps about irregularly, (ii) the real component is much too large for the higher order phases, (iii) the imaginary component is always much too large. Errors of type (i) are due to the marked difference in wavelength inside and outside the potential well; thus, in the extreme case of zero incident energy, a phase of given order jumps discontinuously by multiples of π as KR is increased through successive half-integral multiples of π. Errors of type (ii) are due to the exterior wave functions for the larger l having no longer an oscillatory character in the region of the edge of the potential well, but an exponential character. Errors of type (iii) arise from the same

general feature of a considerable difference in the shape of the wave function inside and outside the nucleus; they will be discussed in more detail later.

We should expect to eliminate these types of error for a nucleus with a sharp boundary by fitting the interior WKB wave function onto the exterior wave function. This gives

$$Br^{-1}\sin(\theta+i\xi)=\cos\eta\, j_l(kR)+(-)^l\sin\eta\, j_{-l}(kR), \quad \ldots. \quad (9)$$

and a similar equation in the derivatives, from which to eliminate the constant B and obtain an improved value for the phase η. Values so obtained are given in the fourth column of Table 1. Their close agreement with the exact values justifies the approximations made in deriving the formula (8) and confirms the reasons given for the failure of this formula.

Values obtained with the Born approximation are also shown in the table for comparison. They are seriously in error, even when the phases are small, when the approximation is best.

IV. Application to a Nucleus with a Diffuse Surface

The exact solution for a constant potential is relatively simple, and the calculations of the previous section were merely for a preliminary test of the WKB method. For a non-uniform potential, however, exact calculation of phases involves lengthy numerical integration of the pair of coupled differential equations into which the radial equation separates when u and V are complex. If the WKB method could be used, it would certainly be much quicker.

The form of non-uniform potential tried was

$$\left.\begin{aligned} V&=V_0, && r<R-a;\\ &=V_0(R+a-r)/2a, && R-a<r<R+a;\\ &=0, && R+a<r; \end{aligned}\right\} \quad \ldots. \quad (10)$$

i.e. V falling linearly to zero over a distance $2a$ at the nuclear surface. Values of $2a/R$ of 0·2, 0·4, and 0·6 were taken, also the value 0·2 with a Woods-Saxon tail added; and the incident energy and maximum well depth were as in Section III.

As for a constant potential, large discrepancies were again found between the exact phases and those calculated from (8). The equation (9) with the amplitude factor $P^{-\frac{1}{2}}$ included on the left-hand side was applied at the edge $r=R+a$ of the nucleus, but this procedure did not improve the accuracy of the phases obtained. The reason is that while the phase of the real component of the interior wave function is given fairly well by $\theta+i\xi$, the variation of amplitude is given poorly by the factor $P^{-\frac{1}{2}}$. The improvement on the WKB method due to Bailey (1954) was tried, which for our problem gives

$$u=\exp(-\tfrac{1}{2}p'p^{-1})\sin(p^2-\tfrac{1}{4}p'^2p^{-2})^{\frac{1}{2}},$$

where $p^2=U+iW$, and which obviously reduces to the usual WKB formula for $p'=0$. This wave function was fitted at the boundary $r=R+a$ to the exterior wave function, but the accuracy of the phases so obtained was not greatly

improved. Inspection of the values of u_r and u_i obtained by numerical integration showed that the approximation $\chi=\varphi$ made in Section I is poor for a varying potential, and that the phase is extremely sensitive to the shape of the wave function just inside the nuclear surface—much more so than for V real. A highly accurate interior wave function is required, and any iterative or other method of finding it with sufficient accuracy would be almost as laborious as numerical integration of the wave equation.

V. Energy-dependent Fluctuations in the Phase Shift

In view of the unexpectedly large fluctuations of the phases about the approximate WKB values, especially of the imaginary component, the energy variation of the phase was investigated over the energy range 0–140 MeV. The zero order phase for a square well (with the same radius as in Section III) was studied for simplicity. The formula (**6**) without the Langer modification then reduces to

$$\eta_0=(K-k)R,$$

while the exact value of η_0 is given by

$$\tan(\eta_0+kR)=(kR/KR)\tan KR.$$

V_i was increased regularly from 3 to 15 MeV over the energy range (Lane and Wandel 1955), and V_r kept constant at 42 MeV.

The exact values of η_r and η_i, the real and imaginary components of η_0, are graphed in Figure 1 as a function of $E^{\frac{1}{2}}$, and are seen to oscillate violently above and below the WKB values in a characteristic way. This behaviour may be understood through the following picture. Let us represent u_r and u_i by displacements in the x and y directions respectively, and r by distance along the z axis. Then from (**5**) the interior wave function is an expanding spiral with Oz as axis, flattened so as to be thinner in the y direction. The exterior wave function, $\sin(kr+\eta_r+i\eta_i)$, is a helix with Oz as axis, flattened in the same direction, the ratio of the widths of the helix in the y and x directions being $\tanh\eta_i$. At low energies the z-distance between successive loops of the helix is much larger than the z-distance between successive loops of the spiral. Fitting the spiral and the helix together smoothly at the boundary thus involves a double requirement, which is usually met only by a stretching of the helix in either (*a*) the x direction, (*b*) the y direction, or (*c*) some intermediate direction. Case (*a*) occurs when u_r is near a zero and u_i near a maximum at the boundary, and corresponds to a diminished value of $\tanh\eta_i$. Case (*b*) is the reverse, and corresponds to an increased value of $\tanh\eta_i$: this is a resonance effect, which gives values of $\tanh\eta_i$ up to 1 (large η_i). Large changes occur simultaneously in η_r. A resonance effect occurs also for purely real potentials, as shown by the dotted curve for η_r, obtained by an exact calculation with K real; but the fluctuations in the curve are much less violent.

A similar effect is to be expected for higher order phases, so long as the exterior wave function is still oscillatory.

The effect of rounding off the potential at the boundary does not affect the general behaviour shown in Figure 1. Thus the dot-dash curve, obtained by numerical integrations for the potential (**10**) with $2a/R=0\cdot4$, exhibits just as marked a resonance effect as the curve for a square well. The occurrence of the resonance at a lower energy is due merely to the effective mean radius for potential (**10**) differing from the average value R. However, rounding off the

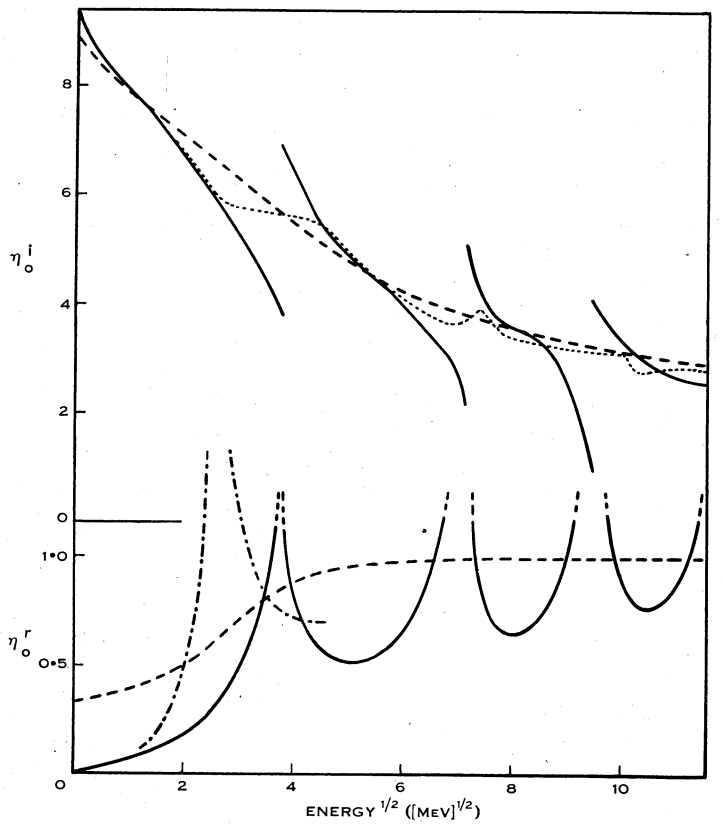

Fig. 1.—Energy dependence of the real and imaginary parts of the zero order phase shift, for neutrons incident on a nucleus of mass number 100.

——— Exact, for square well, complex potential;
- - - - - WKB, for square well, complex potential;
····· Exact, for square well, real potential;
·—·—· Exact, for well of form (**10**) with $2a/R=0\cdot4$, complex potential.

potential brings the values of η_i around a minimum nearer to the WKB value; an effect which is due to the interior and exterior solutions fitting together more readily when there is a finite region over which the alteration from spiral to helical form can take place.

For α-particles, much larger values of V_i are required to match the greater absorption in nuclear matter (Mohr and Robson 1956). The interior wave function is then a very rapidly expanding spiral, and the increased difficulty

of fitting it to the exterior wave function will produce in general a very greatly diminished value of η_i, unless the potential well is rounded off near the edge. For a square well, increasing V_i causes η_i to increase first to a maximum and then decrease to smaller and smaller values.

For high energy nucleons, the values of η fluctuate much less about the WKB values, and also many phases contribute to the scattering cross section, so that the fluctuations largely cancel each other out and produce little effect. The WKB method may therefore be used at intermediate and high energies, the region of validity depending on the size of the nucleus and on the final accuracy required. The number of phases effective in scattering is of the order of $K_r R$, and the magnitude of this quantity will be a rough indication of the accuracy of cross sections calculated with the WKB method. The method need not, of course, be restricted to the case considered here of the same radial dependence of V_r and V_i.

The significance of the results of calculations that have now been carried out for many nuclei at energies of only a few MeV with a square well is limited somewhat on account of the sensitivity of the calculated results to the form of the potential near the nuclear surface. A square well is not a realistic form of potential to adopt.

VI. References

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