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THE SHORT WAVELENGTH APPROXIMATION
TO THE SCHRÖDINGER EQUATION ⁺⁾

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ABSTRACT

We study the short wavelength approximation to the Schrödinger equation in the presence of one and two turning points. Two methods are presented which allow the evaluation of the higher corrections to the elementary W.K.B. approximation. The first method, the "real method" employs higher transcendental functions, the second one uses complex integration techniques.

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I. INTRODUCTION

The small wavelength approximation for the Schrödinger equation is a very useful tool for the study of bound states and scattering problems. Very frequently this method leads rapidly to a simple understanding of the physical situation. Therefore the problem of computing the higher order terms in the small wavelength expansion is certainly very interesting because it gives an estimate of the degree of validity of the semi-classical approximation.

There is, however, a difficulty coming from the presence of the so-called turning points, i.e., those points where the classical velocity is zero, and consequently the wavelength infinite. It is not surprising that the higher order corrections do diverge very badly in those points.

The small wavelength approximation method can be treated in two different ways :

- a) one can write the wavefunction $\psi(x)$ as

$$\psi(x) = e^{\lambda \int^x g(x') dx'} ;$$

one obtains for $g(x)$ a Riccati differential equation, which can be solved with a perturbative expansion;

- b) one can perform a suitable change of variable in such a way that this part of the resulting equation, which contains the parameter λ^2 , can be solved exactly.

Both these approaches can be used in an elementary way, at the price to encounter divergent integrals. In order to overcome this difficulty the two procedures have been applied in the following way.

In the first case one continues the wave function $\psi(x)$ in the complex plane ¹⁾. This method, whose origin can be found already in the paper by Wentzel ²⁾, has been then developed by Dunham ³⁾, Kemble ⁴⁾ and Bottino et al. ⁵⁾. In particular (see section IV) already in Wentzel's original paper one finds for the

bound state problem the right formula for the corrections to first order approximation, which has been after justified in a more rigorous way.

This method, which uses the continuation in the complex plane, can be either extremely simple or (when the maximum mathematical rigour is requested), extremely difficult and makes use of a rather highbrow mathematics (at least in the frame of reference of the present authors).

The second method ⁶⁾ is based on the idea of using a transformation of variables such that one has to do with an equation for higher transcendental functions instead of elementary (exponential) ones, so that the transformation of variables has no more singular points.

Since it does not exist, to our knowledge, in the literature a unified treatment of the problem, that shows the substantial equivalence of the two methods, we have considered it useful to write this paper. Also if this article is in part a rearrangement of published (also if not always well-known !) material, it contains some new results, as for instance the use of the Hermite polynomials in the bound state problem and the general expression for the scattering phase shift.

In section II some well-known features of the classical method will be reported. Section III will deal with the "real method", which, to get the higher order corrections, makes use of higher transcendental functions like Airy functions for scattering and Hermite polynomials for bound states. In section IV we shall use a more direct, although less rigorous method which employs complex path integration.

II. GENERAL FEATURES OF THE CLASSICAL APPROXIMATION

In this paper all our considerations will concern the one-dimensional Schrödinger equation

$$\left\{ \frac{d^2}{dx^2} + 2\mu E - U(x) \right\} \psi(x) = 0 \quad (h = 1) \quad (1)$$

where the variable x runs between $-\infty$ and $+\infty$, and the radial equation for the ℓ^{th} partial wave is

$$\left\{ \frac{d^2}{dr^2} + 2\mu E - U(r) - \frac{\ell(\ell+1)}{r^2} \right\} \chi_\ell(r) = 0 \quad (2)$$

with $0 \leq r < \infty$.

We wish to discuss a method of approximation valid when the "wavelength" $(2\mu E - U)^{-\frac{1}{2}}$ is small if compared to the size of the region where U varies appreciably. In other words we can consider U as constant in a region of the order of magnitude of several "wavelengths". At the end of this paper we shall obtain a more precise and quantitative definition of the "small wavelength approximation".

As we shall see, it is possible to bring also Eq. (2) to a one-dimensional form so that it will be sufficient to focus our discussion on an equation of the form :

$$\left\{ \frac{d^2}{dx^2} + \lambda^2 V(x) \right\} \psi(x) = 0 \quad (3)$$

where

$$\lambda^2 V = 2\mu E - U = k^2 - U \quad (4)$$

λ^2 is a parameter which has been introduced as a device to count correctly the order of approximation.

There are several situations for which a classical-like approximation can be useful. First of all when the potential U is either very large (strong coupling limit) or slowly varying with the distance, a classical approximation is also well justified when the kinetic energy becomes very large. In this respect, it is important to remark that (in the three-dimensional case) for regular potentials (i.e., which behave at the origin better than $1/r^2$) the high-energy limit can be easily obtained from the Born series, that is a perturbation expansion in U/E . For singular potentials, however, the Born series breaks down and to get the high-energy limit we have to use the classical approximation. (This point will be discussed in more detail in a subsequent paper.) *)

It is well known that the behaviour of the solutions of Eq. (2) depends on the sign of $V(x)$. For $V(x) > 0$ the solution is of an oscillating type **, whereas for $V(x) < 0$ one finds an exponentially decreasing behaviour. The transition points or turning points where $V(x) = 0$ (simple zeros) are of the greatest importance in our discussion : at these points the small wavelength approximation does indeed break down (since there $1/\lambda \cdot V^{\frac{1}{2}} = \infty$).

The appearance of turning points is a practically unavoidable feature of any problem of physical interest. In fact, if we consider a scattering problem, the scattered wave is due to the reflection at - at least - one turning point. Analogously, in a bound state problem, the existence of a stationary wave requires reflection at two turning points, at least. More generally, we shall see in Section IV that all the general

*) More precisely in this paper we will always consider potentials which satisfy the requirements :

$$\lim_{r \rightarrow 0} r^2 U(r) = 0, \quad \lim_{r \rightarrow \infty} r U(r) = 0$$

**) This is the region classically accessible to the particle and we will call it the "classical region".

features of the classical approximation depend in an essential manner on the location of the turning points in the complex x plane. In this paper we will limit ourselves to the study of one (scattering) and two (bound states) turning points on the real axis.

To get a better insight into the difficulties of the small wave-length approximation, let us develop it in its standard form. We begin by considering the region where $V(x) < 0$. As suggested by the real exponential character of the wave function, we put

$$\psi(x) = e^{\pm z(x)} \quad (5)$$

$$z(x) = \lambda \int^x q(x') dx' \quad (6)$$

with

$$\phi(x) = \sqrt{-V(x)} \quad (\text{real}) \quad (7)$$

We get the Riccati equation

$$q^2 \pm \frac{1}{\lambda} \dot{q} = \phi^2 \quad (8)$$

We introduce the splitting

$$q(x) = a(x, \lambda) + \frac{1}{\lambda} b(x, \lambda) \quad (9)$$

where a and b are even functions in λ . Separation of the even and odd parts in λ gives

$$a^2 = \phi^2 - \frac{1}{\lambda^2} (b^2 \pm \dot{b}) \quad (10)$$

$$b = \mp \frac{1}{2} \frac{\dot{a}}{a} = \pm \frac{d}{dx} \ln a^{-1/2}$$

6.

so that

$$\psi(x) = a^{-1/2} e^{\pm \lambda \int^x a(x') dx'} \quad (11)$$

and the correct combination of the two independent solutions is fixed by the boundary conditions.

Finally, for $a(x)$ we have the non-linear equation :

$$a(x) = \left\{ \phi^2 - \frac{1}{\lambda^2} I_a \right\}^{1/2} \quad (12)$$

$$I_a = a^{1/2} \frac{d^2}{dx^2} a^{-1/2} \quad (13)$$

Equations (10) and (13) are the starting point for the iteration method. In fact, putting

$$a(x, \lambda) = a_0(x) + \frac{1}{\lambda^2} a_1(x) + \frac{1}{\lambda^4} a_2(x) + \dots$$

one finds

$$\begin{aligned} a_0 &= \phi \\ a_1 &= -\frac{1}{2} a_0^{-1/2} \frac{d^2}{dx^2} a_0^{-1/2} = -\frac{1}{2} \phi^{-1/2} \frac{d^2}{dx^2} \phi^{-1/2} \\ a_2 &= -\frac{1}{8} \left\{ a_1 a_0^{-3/2} \frac{d^2}{dx^2} a_0^{-1/2} - a_0^{-1/2} \frac{d^2}{dx^2} a_1 a_0^{-3/2} \right\} \\ &\quad - \frac{1}{8} \phi^{-2} \left[\frac{d^2}{dx^2} \phi^{-1/2} \right]^2 \end{aligned} \quad (14)$$

Analogously

$$b(x, \lambda) = b_0(x) + \frac{1}{\lambda^2} b_1(x) + \frac{1}{\lambda^4} b_2(x) + \dots$$

and

$$b_0 = \mp \frac{1}{2} \frac{\dot{a}_0}{a_0} = \mp \frac{1}{2} \frac{\dot{\phi}}{\phi}$$

$$b_1 = \mp \frac{1}{2} \frac{d}{dx} \left(\frac{a_1}{a_0} \right) \quad (15)$$

$$b_2 = \mp \frac{1}{2} \frac{d}{dx} \left(\frac{a_2}{a_0} - \frac{1}{2} \frac{a_1^2}{a_0^2} \right)$$

In the same way, we can discuss the region where $V(x) > 0$. Here ϕ becomes purely imaginary and as a consequence a becomes imaginary $a = i\alpha$, b remains real. Thus, for the wave function, we can write :

$$\psi(x) = e^{\pm \zeta(x)} \quad (5')$$

$$\zeta(x) = \lambda \int^x \gamma(x') dx' \quad (6')$$

and

$$\gamma^2 \pm \dot{\gamma}/\lambda + V = 0 \quad (8')$$

To separate the real and imaginary parts, we write :

$$\gamma(x) = i\alpha(x, \lambda) + \frac{1}{\lambda} \beta(x, \lambda) \quad (9')$$

and from (8') we have the equivalent system

$$\beta(x) = \mp \frac{1}{2} \frac{\dot{\alpha}}{\alpha} = \pm \frac{d}{dx} \ln \alpha^{-1/2} \quad (10')$$

$$\alpha^2 = V + \frac{1}{\lambda^2} (\beta^2 \pm \dot{\beta}) = V + \frac{1}{\lambda^2} \alpha^{1/2} \frac{d^2}{dx^2} \alpha^{-1/2} \quad (12')$$

The wave function is now

$$\psi(x) = \alpha^{-1/2} e^{\pm i\lambda \int^x \alpha(x') dx'} \quad (11')$$

and, as is well-known, α contributes to the phase and β to the absolute value.

Starting from Eqs. (10') and (12') we can get for the different iterations expressions analogous to the previous ones. Clearly, the crucial feature of the problem is to join the two previous expansions through the turning points. This has been attempted in many ways. For instance, one can develop $V(x)$ around the turning points and find there an approximate expression for the wave function. However, the final results are not of simple application. It will be shown in Section IV how formulae (11) and (15) can be still used to get convergent expressions for the phase shifts and the bound state condition.

It is important to study the behaviour of the different terms of the series for a and b in the neighbourhood of a turning point x_0 . There $V(x) \sim x_0 - x$

$$a_0 \sim (x - x_0)^{1/2}, \quad a_1 \sim (x - x_0)^{-5/2}, \quad a_2 \sim (x - x_0)^{-9/2}, \dots$$

$$b_0 \sim (x - x_0)^{-1}, \quad b_1 \sim (x - x_0)^{-4}$$

and in general

$$a_m \sim (x - x_0)^{1/2 - 3m}, \quad b_m \sim (x - x_0)^{-(1 + 3m)} \quad (16)$$

Therefore we see that all the integrals of the form $\int a_n dx$ (except $\int a_0 dx$) are badly divergent, the worst the higher the order. The appearance of these infinities makes the elementary application of the classical approximation hopeless.

We want also to investigate the asymptotic behaviour of the iteration scheme when $x \rightarrow \pm\infty$. We observe that in any case $V(x)$ goes, at $x \rightarrow \pm\infty$, never better than a constant, owing to the k^2 term [Eq. (4)]. Otherwise, if the potential diverges at the boundaries, $V(x)$ is in these regions an increasing function of x . However, just from the

fact that ϕ never vanishes for $x \rightarrow \pm\infty$, we see by explicit inspection of Eqs. (14) and (15) that asymptotically the only important terms are a_0 and b_0 (also if b_0 vanishes, the other iterations vanish more rapidly) *).

This is a quite important point : first of all it guarantees that already the lowest order approximation satisfies the right boundary conditions. Secondly it shows that the standard iteration procedure, through exponentials, is particularly good in the asymptotic region where it reproduces quite well the wave function. We will come back to this point in Section IV. To conclude this Section we want to show how to transform the radial problem (2) in a one-dimensional Schrödinger equation (1). In addition, besides the formal manipulations, this will enable us to recognize some features of the problem.

Our purpose can be attained changing the variable $r \rightarrow x$, so that $r \rightarrow 0$ corresponds to $x \rightarrow -\infty$. To do this we put ⁷⁾

$$r = e^x \quad (17)$$

and with

$$\chi_\ell(r) = r^{1/2} \psi_\ell(r) \quad (18)$$

we find that ψ_ℓ satisfies

$$\left\{ \frac{d^2}{dx^2} + \lambda^2 V(x) \right\} \psi_\ell(x) = 0 \quad (19)$$

where

$$\lambda^2 V(x) = e^{2x} [k^2 - U(e^x)] - (\ell + 1/2)^2 \quad (20)$$

*) To fix the ideas, let us consider an explicit example :
 $V(r) = \left\{ k^2 - U(r) - L^2/r^2 \right\}^{1/2}$ where $U(r)$ is regular and short range. As $r \rightarrow \infty$, $V \sim k$, $a_0 \sim c_1 + c_2/r^2$, $a_1 \sim 1/r^4$, $b_0 \sim 1/r^3$, $b_1 \sim 1/r^5$.

Equation (20) shows the "W.K.B. rule" $\ell(\ell+1) \rightarrow (\ell + \frac{1}{2})^2$. Evidently we can apply to Eqs. (19) and (20) all the previous results which are summarized in Eqs. (5)-(13). In particular we can rewrite Eq. (13) in the variable "r". We get

$$I_a = r^2 a^{1/2} \left(\frac{d^2}{dr^2} + \frac{1}{r} \frac{d}{dr} \right) a^{-1/2} \quad (21)$$

Introducing

$$\bar{a}^{-1/2} = r^{1/2} a^{-1/2} \quad (22)$$

Eq. (12) becomes

$$\bar{a} = \left\{ \bar{\phi}^2 - \frac{1}{\lambda^2} I \bar{a} \right\}^{1/2} = \left\{ \bar{\phi}^2 - \frac{1}{\lambda^2} \bar{a}^{1/2} \left(\frac{d^2}{dr^2} + \frac{1}{4r^2} \right) \bar{a}^{-1/2} \right\}^{1/2} \quad (23)$$

$$\lambda^2 \bar{\phi}^2 = - \left[k^2 - v(r) - \frac{(\ell + 1/2)^2}{r^2} \right]$$

so that

$$\begin{aligned} \chi_\ell(r) &= r^{1/2} \psi_\ell(r) = r^{1/2} a^{-1/2} e^{\pm \lambda \int^r a(x') dx'} = \\ &= \bar{a}^{-1/2} e^{\pm \lambda \int^r \bar{a}(r') dr'} \end{aligned} \quad (24)$$

and we notice from this that if we would like to apply the W.K.B. method directly to Eq. (2), we would have to use the modified $\bar{\phi}^2$ and to introduce the "counter term" $+1/4r^2$ (which has the role, as it can be easily verified, to make $I\bar{a}$ finite at $r=0$).

The reason for this is the following: the form of the W.K.B. solution is symmetric (in the sense that $\psi = e^{\pm iZ(x)}$) while, for instance, the behaviour of $\chi_\ell(r)$ at the origin is

$$\chi_\ell(r) \sim r^{\ell+1}, r^{-\ell}$$

which has not this property. To gain this symmetry we introduce

$$\psi_\ell(r) = r^{-1/2} \chi_\ell(r)$$

which indeed behaves

$$\psi_\ell(r) \sim r^{\pm(\ell+1/2)} \quad (25)$$

and obeys the equation

$$\left\{ \frac{d^2}{dr^2} + \frac{1}{r} \frac{d}{dr} + r^2 - \ell(\ell+1) - \frac{(\ell+1/2)^2}{r^2} \right\} \psi_\ell(r) = 0 \quad (26)$$

If we want now to eliminate the first derivative, we can introduce the variable $x = \ln r$ because

$$\frac{d^2}{dr^2} + \frac{1}{r} \frac{d}{dr} = \frac{1}{r^2} \frac{d^2}{d(\ln r)^2}$$

and this gives back our previous result.

From a more physical point of view, we can say that in the three-dimensional problem the appropriate variable is not r but $\ln r$. In fact it restores, in a certain sense, the symmetry between the two boundaries attaching the same importance to $r=0$ and $r=\infty$.

A problem which is still to be discussed is what happens when the potential is such that only a part of it is large

$$\lambda^2 V = \lambda^2 V_0 + \delta V$$

In this case one can rearrange the iteration method by counting in a different way the orders in λ^2 .

We want to notice, however, that this separation is possible only when the part δV of the potential does not influence the behaviour of the wave function at the boundaries.

For instance if the potential is

$$\lambda^2 V = \lambda^2 (1 + k^2 - \ell(\ell+1)/r^2)$$

even if λ^2 is large, it is neither allowed to iterate in k^2 , since this term gives the behaviour at large distances, nor in the centrifugal term $\ell(\ell+1)/r^2$, which gives the behaviour at the origin.

The previously discussed procedure shows how to take into account the centrifugal potential in a non-perturbative way.

The situation looks very different when one has to do with potentials singular at the origin. In this case the centrifugal term does not enter into the behaviour at the origin and can therefore be treated as a perturbation⁸⁾.

Thus for singular potentials [see the following paper⁹⁾] the transformation (17) is not necessary and one can directly apply the "small wavelength approximation" to the original equation (2).

III. THE REAL METHOD

In this Section we want to discuss the application of the real method to scattering and bound states. This method is essentially based on the idea of reexpressing the Schrödinger equation in a new variable such that the large λ^2 limit can be computed exactly, this limit leads to the well-known W.K.B. expression. It is possible, starting from this term, to construct a series of successive approximations.

In III.1 we shall discuss the general features of the method which will be applied to scattering in III.2 and to bound states in III.3. The results for higher order terms are still in an implicit form involving integrals on functions, both of the new and old variables. In III.4 we shall see how this practical difficulty can be overcome and can give explicit expressions for the corrections to W.K.B.

The real method has the advantage of great generality but it becomes soon rather cumbersome as the order of the approximations goes up. Therefore we shall limit ourselves to the next significant correction to W.K.B. The higher order terms can be obtained much more quickly and simply by means of the method discussed in Section IV.

III.1 The Langer procedure

We start from the differential equation

$$\left\{ \frac{d^2}{dx^2} + \lambda^2 V(x) \right\} \psi(x) = 0 \quad (1)$$

where the variable x is real and runs between $-\infty$ and $+\infty$. The coefficient $V(x)$ will be supposed to satisfy all the necessary requirements of continuity and differentiability. $V(x)$ can present a finite number of simple zeros on the real axis (turning points). In this paper we shall concentrate on the case of one or two real turning points.

We introduce a new variable $y(x)$ defined by

$$\frac{dy}{dx} = \alpha \quad (2)$$

and Eq. (1) becomes

$$\left\{ \frac{d^2}{dy^2} + \lambda^2 \left(\frac{V}{\alpha^2} + \frac{I}{\alpha^2} \right) \right\} \varphi(y) = 0 \quad (3)$$

where

$$\varphi(y) = \alpha^{1/2} \varphi(x) \quad (4)$$

and

$$I = -\alpha^{-3/2} \frac{d^2}{dy^2} \alpha^{1/2} = \alpha^{1/2} \frac{d^2}{dx^2} \alpha^{-1/2} \quad (5)$$

We take

$$\frac{V(x)}{\alpha^2} = u_0(y) \quad (6)$$

i.e.,

$$\frac{dy}{dx} = \alpha = V^{1/2}(x) u_0^{-1/2}(y) \quad (6')$$

In this manner, Eq. (3) becomes

$$\left\{ \frac{d^2}{dy^2} + \lambda^2 u_0(y) + \frac{I}{\alpha^2} \right\} \varphi(y) = 0 \quad (7)$$

Let us discuss the meaning of the function $u_0(y)$. In the elementary approach to the W.K.B. approximation, one would have taken $u_0(y)=1$, so that in the large λ limit Eq. (7) would have a simple exponential solution. Here we shall make use of the freedom in the choice of $u_0(y)$ by requiring $u_0(y)$ to vanish at the turning points in such a way that α as given by Eq. (6') tends in those points to a non-vanishing finite limit.

The importance of this requirement can be understood by looking at the expression for I [Eq. (5)]. It is easily seen that if $\alpha(x)$ behaves at $x=x_0$ like $(x-x_0)^{\frac{1}{2}}$ at this point one has $I(x) \sim 1/(x-x_0)^2$ so that a perturbative expansion in I necessarily gives divergent integrals. From Eq. (6') we observe that if the effect of the branch point of $V^{\frac{1}{2}}(x)$ is compensated by the factor $u_0^{-\frac{1}{2}}(y)$ so that α has no branch point, I is finite at $x=x_0$ and a perturbation method can be applied.

On the other hand, $u_0(y)$ has to be simple enough so that the limit for large λ of Eq. (7) can be explicitly obtained in terms of known functions. This can be done in terms of hypergeometric functions if $u_0(y)$ is a second degree polynomial in y . This is the reason why we limit ourselves to only two real turning points.

From Eq. (6') we get the implicit relation

$$\int_{y_1}^y u_0^{1/2}(y') dy' = \int_{x_1}^x V^{1/2}(x') dx' \quad (8)$$

where x_1 and y_1 are zeros of $V(x)$ and $u_0(y)$, respectively.

If there is another turning point x_2 we have to require

$$\int_{y_1}^{y_2} u_0^{1/2}(y') dy' = \int_{x_1}^{x_2} V^{1/2}(x') dx' \quad (8')$$

giving a constraint in the parameters appearing in $u_0(y)$. In the following treatment, it will be useful to have $u_0(y)$ as a function of the parameter λ^2 , writing :

$$u_0(y) = u(y) - \frac{1}{\lambda^2} \omega(\lambda^2) \quad (9)$$

so that with this last definition Eq. (3) can be written :

$$\left\{ \frac{d^2}{dy^2} + \lambda^2 u(y) + F(y) \right\} \varphi(y) = 0 \quad (10)$$

with

$$F(y) = \frac{I}{\alpha^2} - \omega(\lambda^2) \quad (11)$$

and $F(y, \lambda)$ can be expressed in the form :

$$F(y, \lambda) = f_0 + \frac{1}{\lambda^2} f_1 + \frac{1}{\lambda^4} f_2 + \dots = \sum_{v=0}^{\infty} \frac{f_v(y)}{\lambda^{2v}}$$

Let us consider now the equation

$$\left\{ \frac{d^2}{dy^2} + \lambda^2 u(y) \right\} \varphi_0(y) = 0 \quad (12)$$

and φ_0 a solution of it, determined by the boundary conditions of the particular problem considered.

Following Langer ⁶⁾, we take

$$\varphi(y) = A(y, \lambda) \varphi_0(y) + \frac{1}{\lambda^2} B(y, \lambda) \dot{\varphi}_0(y) \quad (13)$$

Using Eq. (12) and the corresponding expression for $\dot{\varphi}_0$

$$\frac{d^2}{dy^2} \dot{\varphi}_0 + \lambda^2 (\dot{u} \varphi_0 + u \dot{\varphi}_0) = 0 \quad (12')$$

equation (10) becomes

$$(\ddot{A} - 2\dot{B}u - B\dot{u} + AF) \varphi_0 + \left(2\dot{A} + \frac{FB}{\lambda^2} + \frac{\ddot{B}}{\lambda^2}\right) \dot{\varphi}_0 = 0$$

or

$$\left. \begin{aligned} \ddot{A} + FA - 2\dot{B}u - B\dot{u} &= 0 \\ 2\dot{A} + \frac{1}{\lambda^2} (\ddot{B} + BF) &= 0 \end{aligned} \right\} \quad (13)$$

This pair of equations can be formally integrated

$$A = -\frac{1}{2\lambda^2} \int_{\bar{y}}^y [\ddot{B} + BF] dy' + 1 \quad (14)$$

$$B = \frac{1}{2} u^{-1/2} \int_{\bar{y}}^y u^{-1/2} [\ddot{A} + FA] dy' = u^{-1/2} C \quad (15)$$

$$C = \frac{1}{2} \int_{\bar{y}}^y u^{-1/2} [\ddot{A} + FA] dy' \quad (15')$$

where we have normalized A by requiring $A=1$ at the lowest order in $1/\lambda^2$.

Equations (15) and (15') show a very important feature : because of the factor $u^{-1/2}$ outside of the integral, B diverges like $(y-\bar{y})^{-1/2}$ at each zero $\bar{y}$ of $u(y)$ [these zeros differ for $1/\lambda^2$ terms from the turning points]. In order to avoid this divergence, one has to

require that the lower limit of integration in y coincides with $\bar{y}$. If there is more than one zero of $u(y)$, then the regularity requirement leads to the constraint $C(\bar{y}_2) = 0$.

One sees here the close analogy of this discussion with the requirements fixing the limits in Eqs. (8) and (8').

We can now write $A(y, \lambda)$, $B(y, \lambda)$ (and consequently φ) as a sum of successive corrections in $1/\lambda^2$,

$$\begin{aligned} A(y, \lambda) &= 1 + \sum_{\nu=1}^{\infty} \frac{a_{\nu}(y)}{\lambda^{2\nu}} \\ B(y, \lambda) &= \sum_{\nu=0}^{\infty} \frac{b_{\nu}(y)}{\lambda^{2\nu}} \end{aligned} \quad (16)$$

where "n" fixes the order of the approximation. The lowest order approximation gives ($\nu = 0$)

$$a_0 = 1$$

$$b_0(y) = \frac{1}{2} u^{-1/2} \int_{\bar{y}}^y u^{-1/2} f_0 dy' \quad (17)$$

For the successive approximations we have the recurrence formulae

$$\begin{aligned} a_{\nu}(y) &= -\frac{1}{2} \int_{\bar{y}}^y \left[\ddot{b}_{\nu-1} + \sum_{\mu=0}^{\nu-1} b_{\mu} f_{\nu-\mu-1} \right] dy' \\ b_{\nu}(y) &= \frac{1}{2} u^{-1/2} \int_{\bar{y}}^y u^{-1/2} \left[\ddot{a}_{\nu} + \sum_{\mu=0}^{\nu} f_{\nu-\mu} a_{\mu} \right] dy' \end{aligned} \quad (18)$$

with the convention that all the symbols with negative index are zero.

Equations (17) and (18) give the means to get a consistent scheme of approximations for treating any problem of practical interest. In the next Sections we shall study the case of the scattering (one turning point) and of the bound states (two turning points).

III.2 The scattering problem

We now apply the method developed in III.1 to the scattering problem. The partial wave equation (19) [see Eqs. (II.17)~(II.26)] can be written as

$$\left\{ \frac{d^2}{dr^2} + \frac{1}{r} \frac{d}{dr} + k^2 - V(r) - \frac{(l+1/2)^2}{r^2} \right\} \psi_l(r) = 0 \quad (19)$$

or, using the variable $x = \ln r$

$$\left\{ \frac{d^2}{dx^2} + \lambda^2 V(x) \right\} \psi_l(x) = 0 \quad (19')$$

where

$$\lambda^2 V(x) = e^{2x} \left[k^2 - V(e^x) \right] - (l+1/2)^2$$

The boundary conditions for the wave function are :

$$r \rightarrow \infty \quad (\text{i.e., } x \rightarrow +\infty)$$

$$\psi_l(r) \sim r^{-1/2} \sin(kr - 1/2 l\pi + \delta_l) \quad (20)$$

$$r \rightarrow 0 \quad (\text{i.e., } x \rightarrow -\infty)$$

$$\psi_l(r) \sim r^{l+1/2} = e^{(l+1/2)x} \quad (21)$$

Let us now perform the change of variable discussed in III.1. Because we are in the presence of one turning point only, the simplest choice for $u_0(y)$ is

$$u_0(y) = y \quad (22)$$

Putting $y=0$ for $x=x_0$ we get from Eq. (8) :

$$\begin{aligned} \frac{2}{3} \lambda y^{3/2} &= \lambda \int_0^y y'^{1/2} dy' = \lambda \int_{x_0}^x V'^{1/2}(x') dx' = \\ &= \int_{r_0}^r \left[k^2 - u(r') - \frac{(l+1/2)^2}{r'^2} \right]^{1/2} dr'. \end{aligned} \quad (23)$$

In the present case we can choose $u=u_0$ so that $f(y) = 1/\alpha^2$ I. Equation (12) is now

$$\left(\frac{d^2}{dy^2} + \lambda^2 y \right) \varphi_0(y) = 0 \quad (24)$$

and the boundary conditions for $\varphi_0(y)$ are those indicated in Eqs. (20) and (21) : oscillating behaviour at $y \rightarrow +\infty$, exponentially decreasing at $y \rightarrow -\infty$. Equation (24) is the so-called Airy equation, whose regular solution satisfying our boundary conditions is the first Airy function

$$\mathcal{H}_0(y) = \frac{\pi}{3} \left[\left(\frac{\lambda}{3} \right)^{2/3} y \right]^{1/2} \left\{ J_{1/3} \left[\frac{2}{3} \lambda y^{3/2} \right] + J_{-1/3} \left[\frac{2}{3} \lambda y^{3/2} \right] \right\} \quad (25)$$

its behaviour at the boundaries is

$$\mathcal{H}_0(y) \sim \sqrt{\pi} (3^{4/3} \lambda^{2/3} y)^{-1/4} \sin \left[\frac{2}{3} \lambda y^{3/2} + \pi/4 \right] \quad y \rightarrow +\infty \quad (25')$$

$$\mathcal{H}_0(y) \sim \frac{1}{2} \sqrt{\pi} (3^{4/3} \lambda^{2/3} |y|)^{-1/4} \exp \left[- \frac{2}{3} \lambda |y|^{3/2} \right] \quad y \rightarrow -\infty$$

It is useful now to express everything in terms of the original variable r .

To this end we use

$$\begin{aligned} \frac{2}{3} \lambda y^{3/2} &= \int_{r_0}^r \left[k^2 - u(r') - \frac{(l+1/2)^2}{r'^2} \right]^{1/2} dr' = \\ &= \int_{r_0}^r \left\{ \left[k^2 - u(r') - \frac{(l+1/2)^2}{r'^2} \right]^{1/2} - k \right\} dr' + kr - kr_0. \end{aligned} \quad (26)$$

so that asymptotically ($r \rightarrow \infty$)

$$\frac{2}{3} \lambda y^{3/2} \simeq kr + \int_{r_0}^{\infty} \left\{ \left[k^2 - u(r') - \frac{(l+1/2)^2}{r'^2} \right]^{1/2} - k \right\} dr' - kr_0 \quad (26')$$

Finally, in terms of r , the asymptotic form of ψ_0 is

$$\psi_0(r) = \alpha^{-1/2} \varphi_0(y) \simeq r^{-1/2} \sin \left(kr - \frac{1}{2} l\pi + \delta_0 \right) \quad (27)$$

where δ_0 is the classical phase factor of the W.K.B. method

$$\begin{aligned} \delta_0 &= \int_{r_0}^{\infty} dr' \left\{ \left[k^2 - u(r') - \frac{(l+1/2)^2}{r'^2} \right]^{1/2} - k \right\} + \frac{\pi}{2} \left(l + \frac{1}{2} \right) - \\ &- kr_0 = - \int_{r_0}^{\infty} r' \frac{d}{dr'} \left[k^2 - u(r') - \frac{(l+1/2)^2}{r'^2} \right]^{1/2} dr' + \frac{\pi}{2} \left(l + \frac{1}{2} \right). \end{aligned} \quad (28)$$

We can now apply the iteration scheme of III.1^{*)}. We have already seen in Eq. (15) that

$$B = \alpha^{-1/2} C = y^{-1/2} C$$

has a branch point at $y=0$. This can be eliminated by taking the lower limit of integration at $y=0$, i.e.,

$$C = \frac{1}{2} \int_0^y \alpha^{-1/2}(y') [\ddot{A} + FA] dy'.$$

*) It is easy, but important, to recognize that δ_0 vanishes when $u=0$.

From Eqs. (14) and (15) it can be easily seen that A and C have a finite limit as $x \rightarrow +\infty$,

$$\begin{aligned} A(\infty) &= 1 - \frac{1}{2\lambda^2} \int_0^\infty \left[\ddot{B} + \frac{I}{\alpha^2} B \right] dy \\ C(\infty) &= \frac{1}{2} \int_0^\infty y^{-1/2} \left[\ddot{A} + \frac{I}{\alpha^2} A \right] dy \end{aligned} \quad (29)$$

To have an expression for the phase shift δ we remember that

$$\alpha = \sqrt{1/2} y^{-1/2}$$

$$\psi(r) = \alpha^{-1/2} \varphi = \sqrt{-1/4} y^{1/4} \varphi(y)$$

and using Eq. (27) we find easily that

$$\varphi(r) \underset{r \rightarrow \infty}{\sim} [A(\infty) \sin(kr + \delta_0) + C(\infty) \lambda^{-1} \cos(kr + \delta_0)]$$

From this it follows that

$$\delta = \delta_0 + \delta' \quad (30)$$

where δ_0 is given by Eq. (28) and

$$\delta' = \text{arctg} \frac{C(\infty)}{\lambda A(\infty)} \quad (31)$$

To the lowest order $[A(y, \lambda) \simeq 1, \text{tg } \delta' \simeq \delta]$ we get

$$\delta' = \frac{1}{2\lambda} \int_0^\infty y^{-1/2} \frac{I}{\alpha^2} dy \quad (32)$$

We can go back to the variable x using

$$dy = \alpha dx, \quad y^{1/2} \propto \sqrt{V}^{1/2}$$

so that (32) becomes

$$\delta' = \frac{1}{2\lambda} \int_{x_0}^{\infty} dx \, I(x) V^{-1/2}(x). \quad (32')$$

III.3 The bound state problem

We start again from the Schrödinger equation (II.1) and we suppose that $\lambda^2 V(x) = k^2 - U(x)$ has two zeros at the points x_1, x_2 . More precisely

$$V(x) \geq 0 \quad x_1 \leq x \leq x_2 \quad (33)$$

$$V(x) < 0 \quad \text{elsewhere}.$$

As a consequence the behaviour at the boundaries is

$$\psi(x) \sim e^{-k_1 x} \quad x \rightarrow +\infty, \quad k_1 = \sqrt{U(+\infty) - k^2} \quad (34)$$

$$\psi(x) \sim e^{k_2 x} \quad x \rightarrow -\infty, \quad k_2 = \sqrt{U(-\infty) - k^2}$$

In this problem there are two turning points, so that as $u_0(y)$ we have to choose the simplest function with two zeros or

$$u_0(y) = \epsilon_0 - 4y^2 \quad (35)$$

Then we have

$$\int_{-\sqrt{\epsilon_0}/2}^y u_0^{1/2}(y') dy' = \int_{x_1}^x v^{1/2}(x') dx' \quad (36)$$

$x \leq x_2$

and from this we see that

$$y(x_1) = -\frac{\sqrt{\epsilon_0}}{2}$$

More explicitly, we get

$$\frac{\epsilon_0}{4} \left\{ \frac{2y}{\epsilon_0} \sqrt{\epsilon_0^2 - 4y^2} + \arccos\left(-\frac{2y}{\sqrt{\epsilon_0}}\right) \right\} = \int_{x_1}^x v^{1/2}(x') dx' \quad (37)$$

and if we require that

$$y(x_2) = \frac{\sqrt{\epsilon_0}}{2}$$

it follows that

$$\frac{\epsilon_0}{4} = \frac{1}{\pi} \int_{x_1}^{x_2} v^{1/2}(x) dx \quad (38)$$

Equation (7) becomes now

$$\left\{ \frac{d^2}{dy^2} + \lambda^2 (\epsilon_0 - 4y^2) + \frac{I(y)}{\alpha^2} \right\} \varphi(y) = 0 \quad (39)$$

and, as it will appear in the following, it is useful to introduce the decomposition

$$u_0(y) = u(y) - \frac{1}{\lambda^2} \omega(\lambda^2) = (\epsilon - 4y^2) - \frac{1}{\lambda^2} \delta \epsilon$$

$$\epsilon_0 = \epsilon - \frac{1}{\lambda^2} \delta \epsilon ; \quad \frac{1}{\lambda^2} \omega(\lambda^2) = \frac{\delta \epsilon}{\lambda^2} = \frac{\epsilon_1}{\lambda^2} + \frac{\epsilon_2}{\lambda^4} \dots \quad (40)$$

and the corresponding equation is

$$\left\{ \frac{d^2}{dy^2} + \lambda^2 (\varepsilon - 4y^2) + F(y) \right\} \varphi = 0 \quad (41)$$

$$F(y) = \frac{I}{\alpha^2} - \delta \varepsilon$$

As the "free" equation we take now

$$\left\{ \frac{d^2}{dy^2} + \lambda^2 (\varepsilon - 4y^2) \right\} \phi(y) = 0 \quad (42)$$

whose solutions vanishing exponentially at the boundaries are the well-known eigenfunctions of the harmonic oscillator. More precisely

$$\phi_m(y) = e^{-\lambda y^2} H_m(\sqrt{2\lambda} y) \quad (43)$$

where the H_n are the Hermite polynomials and

$$\frac{\lambda \varepsilon}{4} = m + \frac{1}{2} = \frac{\lambda}{4} \left(\varepsilon_0 + \frac{1}{\lambda^2} \delta \varepsilon \right), \quad m = 0, 1, \dots \quad (44)$$

If at the zero order in $1/\lambda^2$ we take $\varepsilon \approx \varepsilon_0$, from Eqs. (44) and (38) we derive the well-known W.K.B. formula

$$\lambda \int_{x_1}^{x_2} \sqrt{V(x')} dx' = \pi \left(m + \frac{1}{2} \right) \quad (45)$$

Equation (45) is the condition which, in the quasiclassical model, determines the stationary states of the system.

To derive the corrections to the classical trajectory, we recall that the relation

$$B(y) = u^{-1/2}(y) C = (\epsilon - 4y^2)^{-1/2} C \quad (46)$$

introduces now in $B(y)$, and consequently in the wave function, two branch points at $y = \pm \sqrt{\epsilon}/2$. As usual the first one can be eliminated defining C as

$$C(y) = \int_{-\frac{\sqrt{\epsilon}}{2}}^y dy' u^{-1/2}(y') [\ddot{A} + FA]$$

To get rid of the second, we take advantage of the arbitrariness in the choice of $\delta\epsilon$, to put

$$\int_{-\frac{\sqrt{\epsilon}}{2}}^{\frac{\sqrt{\epsilon}}{2}} u^{-1/2}(y') [\ddot{A} + FA] dy' = 0 \quad (47)$$

In so doing, we derive a condition which enables us to get $\delta\epsilon$ as a function of the parameters of the problem. Finally, if we introduce the expression of $\delta\epsilon$ in the eigenvalue condition (45), we arrive through Eq. (38) to the modified Sommerfeld conditions.

To lowest order, Eq. (47) is

$$\int_{-\frac{\sqrt{\epsilon}}{2}}^{\frac{\sqrt{\epsilon}}{2}} (\epsilon - 4y^2)^{-1/2} [I/\alpha^2 - \epsilon_1] dy = 0 \quad (47')$$

where we have made the approximations $\delta\epsilon \simeq \epsilon_1$, $A \simeq 1$.

From this it follows

$$\epsilon_1 = \frac{2}{\pi} \int_{-\frac{\sqrt{\epsilon}}{2}}^{\frac{\sqrt{\epsilon}}{2}} \frac{dy}{\sqrt{\epsilon - 4y^2}} \frac{I}{\alpha^2} \quad (48)$$

Neglecting higher order terms in $1/\lambda^2$, one can take in Eq. (48) $\epsilon \simeq \epsilon_0$ and the new Sommerfeld condition becomes

$$\left\{ \lambda \int_{x_1}^{x_2} v^{1/2}(x) dx + \frac{1}{2\lambda} \int_{-\frac{\sqrt{\epsilon_0}}{2}}^{\frac{\sqrt{\epsilon_0}}{2}} \frac{dy}{\sqrt{\epsilon_0 - 4y^2}} \frac{I}{\alpha^2} \right\} = \quad (49)$$

$$= \left(m + \frac{1}{2}\right) \pi$$

The second integral can be expressed through the variable x , if we remember that

$$dy = \alpha dx \quad \text{and} \quad (\epsilon_0 - 4y^2)^{1/2} \alpha = v^{1/2} dx$$

and Eq. (49) is now

$$\left\{ \lambda \int_{x_1}^{x_2} v^{1/2}(x) dx + \frac{1}{2\lambda} \int_{x_1}^{x_2} \frac{I(x) dx}{v^{1/2}(x)} \right\} = \left(m + \frac{1}{2}\right) \pi \quad (50)$$

III.4 Evaluation of the integrals

The method discussed in the previous Sections allows, in principle, the evaluation of the higher corrections to the standard W.K.B. formulae. However, we point out that there is still a practical difficulty in the explicit evaluation of the integrals of interest. In fact, looking for instance at Eqs. (32) and (50), we observe that the functions to be integrated present - through the definition of I and α - a mixed

dependence on the variables x, y . Of course, we can eliminate one of the two variables using the (implicit) equation (8). However, it is difficult to do this in an analytic form so that it is not easy to have, at the end, simple, explicit, expressions for the results. The aim of this Section is to show how to get rid of this difficulty, writing every integral as the difference of two integrals, the first containing only the x variable, and the second only the y . Let us recall the definitions

$$\frac{dy}{dx} = \alpha = \sqrt{1/2}(x) u^{-1/2}(y) \quad (51)$$

$$I = \alpha^{1/2} \frac{d^2}{dx^2} \alpha^{-1/2} \quad (52)$$

and using Eq. (51), I becomes

$$I = \sqrt{1/4}(x) \frac{d^2}{dx^2} \sqrt{1/4}(x) - \alpha^2 u^{1/4}(y) \frac{d^2}{dy^2} u^{-1/4}(y) \quad (53)$$

Therefore if, for the scattering problem, we introduce expression (53) for I in Eq. (32) for the phase shift, we get

$$\delta' = \frac{1}{2\lambda} \left[\int_{x_0}^{\infty} \sqrt{1/4}(x) \frac{d^2 \sqrt{1/4}(x)}{dx^2} dx - \int_0^{\infty} u^{-1/4} \frac{d^2 u^{-1/4}(y)}{dy^2} dy \right] \quad (54)$$

which shows a complete symmetry between x and y .

More explicitly ($u = y$)

$$\delta' = \frac{1}{2\lambda} \left[\int_{x_0}^{\infty} \sqrt{1/4}(x) \frac{d^2 \sqrt{1/4}(x)}{dx^2} dx - \int_0^{\infty} \frac{5}{16} y^{-5/2} dy \right] \quad (55)$$

We remark that both integrals diverge in the lower limit. But if we remember that, as discussed in III.1, I is finite at the turning points, we see that the separate divergences of the two integrals have to cancel out completely ^{*)}. In other words, the quantity

$$\frac{5}{16} \int_0^{\infty} y^{-5/2} dy$$

introduces just the counter-terms necessary to compensate the divergent part of

$$\int_{x_0}^{\infty} V^{-1/4}(x) \frac{d^2}{dx^2} V^{1/4}(x)$$

($\sim \frac{5}{16} \int_{x_0}^{\infty} x^{-5/2} dx$ near the point x_0). Thus we are left with a finite part, which can be extracted, for instance, through an integration by parts. However, there is a much more elegant and simpler method which consists in considering

$$\int_{x_0}^{\infty} \left(V^{-1/4} \frac{d^2}{dx^2} V^{1/4} - u^{-1/4} \frac{d^2}{dy^2} u^{-1/4} \frac{dy}{dx} \right) dx \quad (56)$$

as a contour integral in the complex plane along the path γ of Fig. 1.

In so doing we take advantage of the fact that the integrand in Eq. (56) considered as a function of the complex variable z has a branch point, of the root square type, at x_0 so that we can cut the plane from x_0 to $+\infty$ and γ can be written as

$$\gamma = \frac{1}{4\lambda} \int_{\gamma} dx \left[V^{-1/4} \frac{d^2 V^{1/4}}{dx^2} - u^{-1/4} \frac{d^2 u^{-1/4}}{dy^2} \frac{dy}{dx} \right] \quad (57)$$

*) This can be checked directly by using the relation between x and y , given by Eq. (23).

Now the second term in the integrand has no singularities other than the branch point at x_0 so that its contribution is zero as long as the path γ does not go through x_0 . Thus finally

$$\delta' = \frac{1}{4\lambda} \int_{\gamma} V^{-1/4}(x) \frac{d^2}{dx^2} V^{-1/4}(x) dx \quad (58)$$

This result confirms the important remark by Caianiello ¹⁰⁾ that it is possible to avoid the introduction of counter terms if we define in a convenient way the integrals of interest. Completely analogous considerations can be drawn in the bound state case. Eq. (49) can be written

$$\frac{\pi}{2} \varepsilon_1 = \int_{x_1}^{x_2} \left(V^{-1/4}(x) \frac{d^2}{dx^2} V^{-1/4}(x) - u^{-1/4}(y) \frac{d^2}{dy^2} u^{-1/4}(y) \frac{dy}{dx} \right) dx \quad (59)$$

Again there is a complete cancellation between the divergences of the two terms at the points x_1, x_2 . If we go to the complex plane, now there are two branch points so that the cut and the path γ are those of Fig. 2, and we arrive for ε_1 to the formula

$$\pi \varepsilon_1 = \oint \left(V^{-1/4}(x) \frac{d^2}{dx^2} V^{-1/4}(x) \right) dx \quad (60)$$

The results of this Section look somewhat surprising. On the one hand, we have shown that the use of higher transcendental functions gives rise to suitable counter terms which make all iterations convergent. On the other hand, we have seen that, at the end of the business, the explicit evaluation of the quantities of interest can be done, forgetting the counter terms and using convenient paths in the complex plane. In so doing the final results are very similar to those given by the higher order iterations of the elementary W.K.B. method, which actually are divergent. In fact, in the conventional procedure, the integrals are done on the real axis while our formulae involve integrations on contours which accurately avoid the singularities. Thus the similarity between our final results and those obtained by the elementary expansion suggests the possibility of still using the simple exponential form of the original W.K.B. method, adding suitable prescriptions to work in the complex plane. This will be done in the next Section.

IV. THE COMPLEX METHOD

In this section, we want to re-examine the elementary approach through exponential functions, described in section II. We have already seen that such an expansion breaks down in the neighbourhood of the turning points whereas far from these points it is well adequate. In other words the elementary expansion leads to an incomplete description of the whole physical phenomenon.

In order to avoid the turning points with their complications one can continue the wave function to complex values of the variable x ; however, if one needs a complete treatment of the wave function, the problem of joining the wave function at the turning points is difficult and will not be discussed here.

If on the contrary we limit our interest to on mass-shell quantities, as for instance phase shifts and bound state energies, one obtains quickly simple expressions for both of those quantities.

In order to clarify the problem, we observe that the general form of the solution will be

$$\psi(x) = A e^{\lambda \int^x q(x') dx'} + B e^{-\lambda \int^x q(x') dx'}$$

The general problem is to obtain the two constants A, B ; this is a difficult problem and requires an advanced mathematics (see, for instance, Refs. 5) and 6)).

There are on the contrary some cases in which one of the two coefficients vanishes a priori; in this case the problem becomes remarkably simpler.

In this case, which is the bound state problem, the method allows to obtain very quickly Wentzel's ²⁾ result, this point is discussed in section IV.1.

We shall then show in section IV.2 that also the scattering problem can be treated with a similar method by applying a well-known relation between the phase shift and the energy levels of a system enclosed in a very large sphere. The corrections to the phase shifts are obtained as an integration over a complex path (for the lowest order they coincide with those obtained by Bottino et al. ⁵⁾).

The results obtained in this way will coincide with those obtained in the previous sections, but this formulation will present some definite advantages.

IV.1 Bound states

Let us discuss the bound states problem :

$V(x)$ has two turning points and there is not loss of generality to put them at $\pm c$. Then

$$\begin{aligned} V(x) > 0 & \quad |x| < c \\ V(x) < 0 & \quad |x| > c \end{aligned} \tag{1}$$

We consider first the real axis region $x < -c$ and we will use Eqs. (5...15) of section II which are valid there. We have

$$\psi(x) = e^{\pm z(x)} \tag{2}$$

$$z(x) = \lambda \int_x^{\infty} q(x') dx'; \quad q(x) = a(x) + \frac{1}{\lambda} b(x) \tag{3}$$

For the first iterations we recall the formulae

$$a_0 = \phi, \quad a_1 = -\frac{1}{2} \phi^{-1/2} \frac{d^2}{dx^2} \phi^{-1/2}, \dots \quad (4)$$

$$b_0 = -\frac{1}{2} \frac{\phi}{\phi}, \quad b_1 = -\frac{1}{2} \frac{d}{dx} \left(\frac{a_1}{a_0} \right), \dots \quad (4')$$

As we can see, all the terms in the iteration scheme depend only on ϕ so that, in order to know the analytic properties of a and b , we have first to find a convenient representation for $\phi(x)$ in the complex plane. Now $\phi(x)$ has a branch point at each turning point and we shall make $\phi(x)$ single valued cutting the complex x plane. Since we wish to preserve the original form of the elementary expansion for $x < -c$ the cuts will be chosen as in Fig. 3 where $\xi_1, \xi_2, \dots, \xi_n$ are other eventual complex turning points.

In so doing we continue $\phi(x)$ from the region $x < -c$ (where it has a real, negative, value) to the cut plane and we get an analytic single valued function. In the same way, if we exclude the cut region, $a(x)$, $b(x)$, as given by their expansion in $1/\lambda^2$, are analytic and single valued functions of x . We remember that at the turning points, $a_n(x)$ has branch points of order $1/2-3$ while $b_n(x)$ has poles of order $(+3n+1)$.

Moreover we recall that in the asymptotic region the only important terms are a_0 and b_0 and thus the $1/\lambda^2$ expansion represents quite well the wave function there. Thus the natural idea is to try to join the two regions $x \ll -c$, $x \gg c$ without going through the turning points or crossing the cuts. In the complex plane this can be easily done along a path which avoids the cut regions. It is well known that if we want to have a detailed knowledge of the wave function everywhere also this procedure encounters many difficulties.

However, if we require only that our method preserves the general properties of the wave function, it is possible to derive the physical information leading to the bound state condition. For the wave function ψ we have to require that

- 1) $\psi(x)$ must go to zero when $x \rightarrow \pm\infty$ on the real axis;
- 2) $\psi(x)$ must be a single valued function of x in the cut plane of Fig. 3.

We begin by disposing of the first condition. Since $\phi(x)$ is negative from $-\infty < x < -c$ and positive from $c < x < +\infty$, z will tend to $\pm\infty$ both for $x \rightarrow \pm\infty$. We shall therefore meet condition 1) by choosing the "-" sign in the exponential of Eq. (1)

$$\psi(x) = e^{-z(x)}$$

Let us discuss the monodromy requirement 2). Even if g is single valued in the domain of Fig. 3, z and ψ are not, because the domain is such that the evaluation of $z(x)$ can be done along several paths, giving in general different results. As a consequence the condition for the single-valuedness of ψ will be

$$\lambda \oint g(x) dx = 2\pi i n \quad (5)$$

where the integration is performed on a closed path surrounding the cut $-c, c$ and n is any integer ($n = 0, \pm 1, \dots$).

Equation (5) represents the most general form of the Sommerfeld condition: as we shall see, in this form, all the higher order integrals can be evaluated without any trouble.

If we split now

$$g(x) = a(x) + \frac{1}{\lambda} b(x)$$

the integral on the b part can be easily evaluated. In fact we remember that [Eq. (II.15)]

$$b(x) = -\frac{1}{2} \frac{\dot{\phi}}{\phi} + \frac{d}{dx} (f_1 + f_2 + \dots)$$

Now, since $f_1, f_2 \dots$ are single-valued functions of x in the cut plane, their contribution to the integral (5) will vanish. So we are left with the contribution of the first part only and we get (the integration is taken in the clockwise sense)

$$\oint b(x) dx = \oint b_0(x) dx = -\frac{1}{2} \oint \frac{\dot{\phi}}{\phi} dx = i\pi \quad *) \quad (6)$$

Finally Eq. (5) can be written in the form

$$\begin{aligned} \lambda \oint a(x) dx &= \lambda \oint \left(a_0 + \frac{1}{\lambda^2} a_1 + \frac{1}{\lambda^4} a_2 + \dots \right) dx = 2\pi i (m - \frac{1}{2}) \quad (7) \\ &= 2\pi i (m + \frac{1}{2}) \quad , \quad m = 0, 1, \dots \end{aligned}$$

Equation (7) is the most convenient and general expression of the bound state condition. One can verify that the first two terms in the expansion of Eq. (7) coincide with those obtained with much more generality and pain in the previous sections **)

*) It is clear that $\dot{\phi}/\phi$ has zero discontinuity along the cut but it has two poles of the form $\sim \frac{1}{2} \frac{1}{x \mp c}$ at the turning points.

**) In order to compare Eq. (7) with (III.60) we recall that the analytic function ϕ defined in this section is equal to $iV^{1/2}$.

The best way to evaluate the corrections (as well as the zero order term) is to try to deform the integration contour pushing it as far as possible from the classical region. The maximum distance we can reach depends on the position of the complex turning points. If those extra turning points are completely absent (like in the case of the harmonic oscillator and hydrogen atom) the contours can be pushed up to infinity where the contribution of the higher order terms does indeed vanish and the bound state condition is

$$\lambda \oint \phi(x) dx = 2\pi i (n + 1/2), \quad n = 0, 1, \dots$$

We therefore understand the reason why the conventional, classical approximation leads to the exact answer in those cases (it reproduces all the energy states of the system, including the ground state)*).

This suggests that, in the general case, if the other turning points are far enough in the complex plane from the classical region, the $1/\lambda^2$ expansion would be quite good and it would be the better the farther the turning points are.

To make this more quantitative we can apply a well-known method¹¹⁾ of treating the effect of complex turning points by means of a power series expansion. We write

$$\lambda \phi = \frac{\lambda}{c^2} (x^2 - c^2)^{1/2} F(x/d) \quad (8)$$

where $F(x/d)$ contains the effect of all the other turning points. The parameters λ and d are chosen in such a way that $F(0) = 1$ and that the power series expansion

*) This does not seem to be sufficiently appreciated. It was first recognized in Ref. 1).

$$F(\xi) = 1 + \xi \dot{F}(0) + \xi^2/2 \ddot{F}(0) \quad (9)$$

has radius of convergence 1.

In other words, if the distance of the turning points of $F(x)$ from the integration region is large when compared with the dimensions of this region ($\sim c$), $F(x)$ does not vary appreciably there so that we can develop it around a convenient point (the origin in our case).

If we introduce (8) in (7) we get for the first two iterations ^{*)}

$$J_0 = \frac{\lambda}{i} \oint a_0(x) dx = \frac{\lambda}{i} \oint (z^2 - 1)^{1/2} F(\gamma z) dz ; \quad \gamma = \frac{c}{d} \quad (10)$$

$$\begin{aligned} J_1 &= \frac{1}{8i\lambda} \oint a_1(x) dx = -\frac{1}{8i\lambda} \oint \phi^{-1/2} \left(\frac{d^2}{dx^2} \phi^{-1/2} \right) dx \\ &= \frac{1}{8i\lambda} \oint \phi^{-1} \left(\frac{d\phi}{dx} \right)^2 dx = \frac{1}{8i\lambda} \oint \phi^{-1} \left(\frac{d^2}{dx^2} \ln \phi \right) dx \\ &= \frac{1}{8i\lambda} \oint \frac{dz}{(z^2 - 1)^{1/2}} F(\gamma z) \left\{ \frac{d^2}{dz^2} \ln(z^2 - 1)^{1/2} + \frac{d^2}{dz^2} \ln F(\gamma z) \right\} \quad (11) \end{aligned}$$

Introducing expansion (9) in Eqs. (10), (11) and closing the integration contour at infinity we get

$$J_0 = \pi\lambda \left[1 + \frac{\gamma^2}{8} \ddot{F}(0) + O(\gamma^4) \right] \quad (12)$$

^{*)} In the derivation of Eq. (11) we have repeatedly used integration by part.

$$J_1 = \frac{\pi \gamma^2}{\lambda} \left[\frac{1}{2} \dot{F}^2(0) - \frac{3}{8} \ddot{F}(0) + O(\gamma^2) \right] \quad (13)$$

The meaning of this expansion is clear. We see that two parameters enter the game : λ describing the "strength" of the potential and γ describing its variation in the region where the classical motion takes place.

We see that the higher order terms do contain higher powers not only of $1/\lambda$ but also of γ so that the validity of the classical expansion depends on the order of magnitude of both parameters.

IV.2 Scattering theory

Let us now apply the method discussed in the previous section to the scattering problem.

To this end we remember the well-known fact that a scattering problem can be formally reduced to the bound state one, enclosing our system in a large sphere of radius R (where the wave ψ assumes already its asymptotic form). The unperturbed (for $U = 0$) levels k_n are given by the condition

$$\sin \left(k_n R - \frac{1}{2} l \pi \right) = 0 \quad (14)$$

i.e.,

$$k_n R = \frac{1}{2} l \pi + m \pi \quad (15)$$

Now the effect of the potential is to change the condition (14) to

$$\sin(k'_m R - \frac{1}{2} l\pi + \delta) = 0 \quad (16)$$

i.e.,

$$k'_m R = m\pi + \frac{1}{2} l\pi - \delta \quad (17)$$

and the scattering phase shift is defined through the limit

$$\delta = \lim_{R \rightarrow \infty} (k_m - k'_m) R = \lim_{R \rightarrow \infty} (m\pi + \frac{1}{2} l\pi - k'_m R) \quad (18) \quad *)$$

Our procedure will be now to compute the levels k'_n by means of a generalization of the method discussed in the previous section and to use Eq. (18) to obtain the phase shift.

We follow now the procedure of the previous section. The domain of analyticity of $\phi(x)$ **) is given in Fig. 4.

*) It is not always easy to have a one-to-one correspondence between the unperturbed and perturbed levels. (This would require our adiabatic switching on of the potential.) Anyway, if there would be an error $\mu\pi$ in the difference $k_n - k'_n$, we would have

$$\delta = \lim_{R \rightarrow \infty} (k_n - k'_n) R + \mu\pi$$

This means that all the phase shifts are defined aside an arbitrary factor $\mu\pi$. However, this ambiguity is not relevant for the experimental data because the S matrix does not change if multiplied by $e^{2i\mu\pi} = 1$.

**) We use the "adimensional" formulation of the radial problem through the variable $x = kR$.

$\phi(x)$ is chosen to be negative from $-\infty$ to x_0 , on the real axis. In the cut domain of Fig. 2, $g(x)$, $a(x)$, $b(x)$ as given by Eq. (3) will be analytic and single valued. For what concerns the wave function ψ , the condition $\psi \rightarrow 0$ for $x \rightarrow -\infty$ [which corresponds to choose the regular solution for $r \rightarrow 0$] requires the minus sign in Eq. (II.5).

$$\psi(x) = e^{-z(x)} \quad (19)$$

$$z(x) = \lambda \int^x g(x') dx' \quad (20)$$

We now enclose our system in a large sphere of radius R . The condition which determines the levels of the system is obtained requiring the wave function to be single valued on that surface. In other words we require

$$\frac{\psi^+(R)}{\psi^-(R)} = e^{z(R_-) - z(R_+)} = 1 \quad (21)$$

that is

$$\int_{\gamma(R)} g(x') dx' = 2im\pi \quad m = 0, \pm 1, \dots \quad (22)$$

where the contour γ is shown in Fig. 4.

Equation (22) is the condition for the different levels k'_n *).

In order to get the scattering phase shift by means of the limiting process indicated by Eq. (18) we have to extract from Eq. (22) its explicit dependence on the (large) parameter R . This can be done by isolating in the integrand g the leading term for large (positive) values of x .

*) We remember that k' enters in g through the formula $\phi = \left\{ k'^2 - U(r) - \frac{(l+1/2)^2}{r^2} \right\}^{1/2}$.

$$g = g_0 + g'$$

$$g_0 = a_0 + b_0 \quad (23)$$

$$g' = a' + b' = \sum_1^{\infty} a_i / \lambda^{2i} + \sum_1^{\infty} b_i / \lambda^{2i}$$

Let us evaluate separately those four contributions. We transform the integral on a_0 into the old variable r and perform an integration by parts obtaining

$$\int_{\gamma(x)} a_0(x') dx' = - \int_{\gamma(R)} dr' \cdot r' \frac{d}{dr'} \left[r'^2 - u(r') - \frac{(l+1/2)^2}{r'^2} \right]^{1/2} \quad (24)$$

where the first integral converges when we let $R \rightarrow \infty$.

The integral on b_0 can be easily evaluated (as in the preceding section) by recalling that $b_0 = -\frac{1}{2} \dot{a}_0 / a_0$ is continuous through the cut and presents only a simple pole at x_0 of the form $b_0 \simeq -\frac{1}{4} \frac{1}{x-x_0}$.

Thus we get

$$\frac{1}{2i} \oint b_0(x) dx = \frac{\pi}{4} \quad (25)$$

Finally, introducing Eqs. (24) and (25) in Eq. (22) we find

$$\begin{aligned} m\pi - k'_m R = & - \int_{\gamma(R)} dr' \cdot r' \frac{d}{dr'} \left\{ r'^2 - u(r') - \frac{(l+1/2)^2}{r'^2} \right\}^{1/2} \\ & + \frac{\pi}{4} + \frac{1}{2i} \int_{\gamma(R)} g'(x) dx \end{aligned} \quad (26)$$

Finally, introducing Eq. (26) in the fundamental Eq. (18) and taking the limit $R \rightarrow \infty$, we have

$$\delta = \lim_{R \rightarrow \infty} (n\pi + \frac{1}{2} 2\pi - k'_m R) = \delta_0 + \delta' \quad (27)$$

with

$$\delta_0 = - \int_{r_0}^{\infty} dr' \cdot r' \cdot \frac{d}{dr'} \left[k^2 + U(r') - \frac{(\ell + \frac{1}{2})^2}{r'^2} \right]^{1/2} + \frac{\pi}{2} \left(\ell + \frac{1}{2} \right) \quad (28)$$

$$\delta' = \frac{1}{2i} \int_{\gamma_{\infty}} q'(x) dx \quad (29)$$

where now the contour γ_{∞} is pushed up to infinity.

As in the preceding chapter $b' = \frac{d}{dx} B(x)$ (where $B \rightarrow 0$ when $x \rightarrow \infty$) so that the integral over b' vanishes and we are left with

$$\delta' = \frac{1}{2i} \int_{\gamma_{\infty}} a'(x) dx \quad (30)$$

which is the final expression for the corrections to the classical W.K.B. expression (28) for the phase shift.

V. CONCLUSIONS

In this paper we have discussed the explicit convergent expressions for the higher order corrections to the W.K.B. approximation. The recipe for computing these corrections is to substitute to the divergent integrals appearing in the elementary expansions, analogous integrals on a complex Sommerfeld contour.

One arrives to this simple result in two different ways. The method described in Section III is based on the idea of re-expressing the differential Schrödinger equation in a new appropriate variable. This method leads to a complete and satisfactory (although rather cumbersome one) description of the physical problem, by giving expressions for the wave function valid everywhere.

The difficulties at the turning points are treated by introducing higher transcendental functions. In the explicit calculations, this procedure leads, through the presence of the appropriate counter terms, to the complete cancellation of all infinities. In this way it is possible to express the physical quantities in terms of integrals on the classical path. The thing, however, becomes harder and harder for higher approximations since the number of counter terms quickly increases *).

The method described in Section IV makes use of the non-linear Riccati equation. This method is not adapted to give a complete description of the physical problem since the approximation breaks down at the turning points. However, the application of analytic continuation allows to get quickly the right expressions for bound states and phase shifts in terms of complex integrals.

It is amusing to remark some analogies between the two approaches and the methods applied in field theory.

*) In some way the divergences at the turning points look analogous to the ultra-violet divergences of non-renormalizable theories.

The real method is analogous to the Hamiltonian approach, one makes full use of the linearity of the Schrödinger equation, obtaining expressions for asymptotic as well as non-asymptotic quantities. The infinities (as in the Dyson procedure) are eliminated by means of counter terms which are necessary to make the theory self-consistent. The complex method shows features similar to dispersion theory. One starts from a non-linear equation and concentrates on the asymptotic quantities which are obtained by means of complex integration.

This method leads without needing any counter term to the final results for the "on mass shell quantities".

It is possible that this analogy has a more deep meaning and it might be of use in the understanding of the many dark questions still existing in the treatment of infinities in singular field theories.

RIASSUNTO

Si studia l'approssimazione di piccole lunghezze d'onda per l'equazione di Schrödinger con uno o due punti di transizione. Vengono presentati due metodi che permettono la valutazione delle correzioni alla semplice approssimazione W.K.B. Il primo metodo, il "metodo reale" fa uso di funzioni speciali, mentre il secondo si serve di tecniche di integrazione complessa.

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Fig. (1)

Fig. (2)

Fig. (3)

Fig. (4)