The WKBJ Wavefunctions in the Classically Forbbiden Region: the Connection Formulae

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As well known, the WKBJ approximation method provides an approximate solution to the Schrödinger equation of a quantum mechanical system; but the method fails at the classical turning points (classically forbidden region) of the system's potential energy function. Solutions about these "inaccessible" regions are derived by the transformation of Schrödinger equation to either the Airy or modified Airy differential equation. The asymptotic expansion of these solutions are appropriately connected (connection formulae) with the WKBJ solutions to provide full range solutions and these are used to derive the standard energy level formula (Semiclassical quantization rule), which is applied to obtain the modified semiclassical quantization rule.

1. Introduction

An exact solution of the Schrödinger equation is an impractical proposition except for the simplest of potentials. In most cases of practical interest, one has to settle for an approximate solution. Thus, several methods of approximation have been devised for tackling various types of problems in Quantum mechanics. The asymptotic or WKBJ approximation provides analytical expressions that pave the way for an approximate description of the mechanisms underlying some physical phenomena [1-7]. With it one obtains provision of simple and good approximate solution to the Schrödinger equation that has been widely used for many approximate calculations of quantum mechanical quantities [8-21]. In particular, this approximate method finds useful applications in theoretical nuclear physics [22-24]. The condition for the application of WKBJ approximation is not satisfied at the regions surrounding the classical turning points of the system's potential energy function. However, transformation of the equation of either the Airy or modified Airy differential equation provides more accurate solutions at such inaccessible regions. These solutions are asymptotically extendable to the regions where the WKBJ method is valid, leading to connection formulae.

The purpose of this paper is to present a method for the construction of the WKBJ wavefunctions based on the explicit consideration of matching between the results obtained from the classically allowed and classically forbidden region which is a pure asymptotic approximation technique via the asymptoticity of the Airy and modified Airy functions. These connection formulae are later used to derive the semiclassical quantization condition and also provide its extension to the modified semiclassical quantization

condition. The paper is organized as follows. A brief review of the WKBJ concepts is presented in section 2; section 3 contains the derivation of the connection formulae. Section 4 contains the semiclassical quantization condition, while section 5 contains the conclusion.

2. Review of the WKBJ approximation methods

The principle underlying the method is elucidated in the following way; the stationary wave equation which involves a one-dimensional potential $V(x)$ is

$$\frac{d^2}{dx^2}\Psi(x)+K^2(x)\Psi(x)=0\,,\tag{1}$$

with the local wavenumber

$$K(x)=\left\{\frac{2\mu}{\hbar^2}\Big[E-V(x)\Big]\right\}^{\frac{1}{2}},\text{ if } E>V(x)\tag{2}$$

$$=\left\{\frac{2\mu}{\hbar^2}\big[V(x)-E\big]\right\}^{\frac{1}{2}}=ir(x)\,,\text{ if } E<V(x).\tag{3}$$

If $V(x)=V_0$ (a constant), then equation (1) has solution

$$\Psi(x)=\exp\big(\pm iK_0 x\big)\,,\tag{4}$$

where

$$K_0=\left\{\frac{2\mu}{\hbar^2}\big[E-V_0\big]\right\}^{\frac{1}{2}}.\tag{5}$$

Equation (4) suggests that if $V(x)$ is no longer a constant but varies slowly with x, slow variation of $V(x)$ with x means, that it varies appreciably only over a small distances and it does approximate a constant potential, *i.e.*, $|dV(x)/dx|$ is small, and provided x is not near classical turning point for which we would have $[E - V(x)] = 0$. We may try a solution of equation (1) in the form

$$\Psi(x) = \exp[iu(x)], \tag{6}$$

this converts the linear, time-independent Schrödinger equation for $\Psi(x)$ into the nonlinear Riccati's equation for the function $u(x)$, *i.e.*,

$$i\,u''(x) - [u'(x)]^2 = -K^2(x) \tag{7}$$

The nonlinearity of equation (7) can be used to develop an iteration procedure to obtain the zero-order approximation solution.

$$u_0(x) = \pm \int_0^x K(t)\,dt + C_0, \tag{8}$$

where C_0 is arbitrary constant of integration. Suppose $U_n(x)$ is the nth order iteration, then on re-writing equation(7). Wehave,

$$u_{n+1}(x) = \pm \int_0^x \left[K^2(t) + i\,u_n''(t) \right]^{1/2} dt + C_{n+1}. \tag{9}$$

For $n = 0$, equation (9) gives

$$u_1(x) = \pm \int_0^x \left[K^2(t) \pm iK'(t) \right]^{\frac{1}{2}} dt + C_1. \tag{10}$$

Consequence of this procedure to the correct functions, $u(x)$, demands that $u_1(x)$ should be close to $u_0(x)$. This is possible only if

$$\left| K'(x) \right| << \left| K^2(x) \right|. \tag{11}$$

If condition (11) holds, then Binomial expansion of the integrand in equation (10) gives,

$$u_1(x) \approx \pm \int_0^x K(t)dt + \frac{1}{2} Ln\,[K(x)], \qquad (12)$$

where the constant of integration, C_1, can be absorbed into the normalization of $\Psi(x)$. This first order iteration equation (12) constitutes the WKBJ approximation; and leads to the general approximate wavefunction. By equation (6),

$$\Psi(x) = [K(x)]^{-1/2}\{A\exp[i\int_0^x K(t)dt] + B\exp[-\int_0^x K(t)dt]\}. \quad (13)$$

Whereas in the classically forbidden region (or classically inaccessible region) $E < I_{\min}(x)$, where the wave number $K(x) = ir(x)$. Then, the general approximate wave function $r(x) > 0$ is obtained as,

$$\Psi(x) = [r(x)]^{-1/2}\{A\exp[-\int_0^x r(t)dt] + B\exp[\int_0^x r(t)dt]\} \qquad (14)$$

3.   Derivation of the connection formulae

The validity of equations (13) and (14) depends on the condition (11) being satisfied and by virtue of equations (2) and (3), we have

$$\left| \frac{V'(x)}{2}\left\{ \frac{2\mu}{\hbar^2}[E - V(x)] \right\}^{-\frac{3}{2}} \right| << 1, \qquad (15)$$

according to $E > V(x)$ or vice-versa. Thus, condition(11) breaks either at the classical turning points, where $V(x) = E$, or anywhere $V(x)$ has a very steep gradient, since our iteration procedure already assumed that $V(x)$ varies slowly with x, which implies that $|V'(x)| < 1$, it follows that equations (13) and (14) become invalid around the

classical turning points. Hence, the necessity for another approximate solution of the Schrödinger equation that is valid near a classical turning point. Connection formulae give the correct transfer of the approximate solution valid in the classical region, *i.e.*, $E > V(x)$ or vice-versa. The formulae also depend on whether $V'(x)$ is positive or negative at such turning point. The connection formulae which relate oscillatory and exponential behaviour of the wave forms on the opposite sides of the classical turning points can be matched.
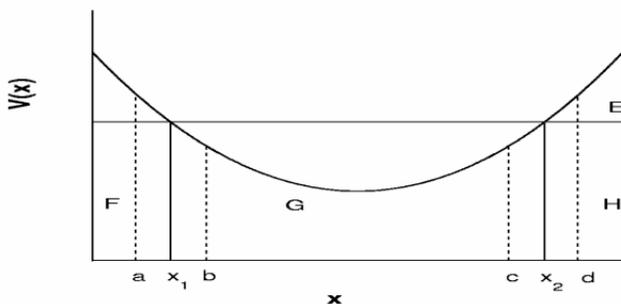
Figure 1: Graph of *V*(*x*) showing the intervals (a, b) and (c, d) around the turning points x_1 and x_2, where WKBJ approximation is valid. F and H are the classically forbidden regions, while G is the classically allowed region.

In Fig. 1, $V(x_1) = V(x_2) = E$, so that the WKBJ approximation is invalid in the interval $a < x < b$ and $c < x < d$, since $V(x)$ is assumed to vary slowly with *x*, we take $V(x)$ to be a linear function of *x* in (a,b) and (c,d); which are respectively neighbourhoods of the turning points x_1 and x_2. For $a < x < x_1$, we expand $V(x)$ in power series about x_1 and retain only the first two terms to give

$$V(x) \approx V(x_1) - (x_1 - x)V'(x) = E + (x_1 - x)F \qquad (16)$$

Where $F = |V'(x_1)|$, equation (16) is the required linear

approximation of $V(x)$ in (a, x_1) and its use in equation (1) gives

$$\Psi''(x) - \frac{2\mu F}{\hbar^2}(x_1 - x)\Psi(x) = 0 . \qquad (17)$$

The substitution

$$\xi = \left(\frac{2\mu F}{\hbar^2}\right)^{\frac{1}{3}}(x_1 - x) , \qquad (18)$$

transforms equation (17) into Airy differential equation

$$\Psi''(\xi) - \xi\,\Psi(\xi) = 0. \quad (19)$$

In a similar fashion, for $x_1 < x < b$

$$V(x) = E - (x - x_1)F. \quad (20)$$

Then, equation (1) becomes

$$\Psi''(\eta) + \eta\,\Psi(\eta) = 0, \quad (21)$$

with

$$\eta = \left(\frac{2\mu F}{\hbar^2}\right)^{\frac{1}{3}}(x - x_1). \qquad (22)$$

Equation (21) is the Modified Airy differential equation and has general solution [25]

$$\Psi(\eta) = A\eta^{\frac{1}{2}}J_{\frac{1}{3}}(\frac{2}{3}\eta^{\frac{3}{2}}) + B\eta^{\frac{1}{2}}J_{-\frac{1}{3}}(\frac{2}{3}\eta^{\frac{3}{2}}) \quad (23)$$

where $J_{\pm n}(\eta)$ are the independent solutions of Bessel's differential equation of order 1/3; with A and B representing the arbitrary constants of integration. From equations (18) and (22), it is easily seen that:

$$\eta = -\xi. \qquad (24)$$

Therefore, the solution of equation (19) is:

$$\Psi(\xi) = \xi^{1/2}\left[-A\,I_{1/3}(\frac{2}{3}\xi^{3/2}) + B\,I_{-1/3}(\frac{2}{3}\xi^{3/2}) \right], \qquad (25)$$

where $I_{\pm n}(x)$ satisfies the Modified Bessel's differential equation of order n. With the use of the asymptotic expansions of $J_n(x)$ and $I_n(x)$ [25, 26] and the facts that $\Psi(\xi)$ must be normalized (for $\Psi(\xi)$ to be normalized, A = B), then, the above equation becomes

$$\Psi(\xi) = B_0\xi^{-1/4}\exp(-\frac{2}{3}\xi^{3/2}), \quad (26)$$

where

$$B_0 = \frac{3B}{2\sqrt{\pi}}, \qquad (27)$$

is an arbitrary constant.

Similarly, putting A = B and using the asymptotic expansion of $J_{\pm n}(x)$ [25, 26] in equation (23) gives

$$\Psi(\eta) = 2B_0\,\eta^{-\frac{1}{4}}Cos\left[\frac{2}{3}\eta^{\frac{3}{2}} - \frac{\pi}{4}\right]. \quad (28)$$

Equations (26) and (28) give the connected formula from region $F(x<x_1)$ (i. e. classically inaccessible region) to region $G(x_1<x)$ with $B_0 = 1$ as

$$\xi^{-\frac{1}{4}}\exp[-\frac{2}{3}\xi^{\frac{3}{2}}]\Big|_{x<x_1} \to 2\eta^{-\frac{1}{4}}Cos\left[\frac{2}{3}\eta^{\frac{3}{2}} - \frac{\pi}{4}\right]\Big|_{x_1<x}.$$

(29)

Now, using equations (16), (18) and (3) in equation (29), we have the connection formula as,

$$[r(x)]^{-\frac{1}{2}}\exp[\;-\int_x^{x_1} r(t)dt] \to 2[K(x)]^{-\frac{1}{2}}Cos\left[\int_{x_1}^x K(t)dt - \frac{\pi}{4}\right],$$

(30)

so also, the second connection formula at x_1 can be obtained as:

$$-[r(x)]^{\frac{1}{2}}\exp[\int_x^{x_1} r(t)dt] \leftarrow [K(x)]^{-\frac{1}{2}}Cos\;\left[\int_{x_1}^x K(t)dt - \frac{\pi}{4}\right].$$

(31)

In the similar manner, the two connection formulae at x_2 are obtained as:

$$2\left[K(x)\right]^{-\frac{1}{2}}Cos\left[\int_x^{x_2}K(t)dt-\frac{\pi}{4}\right]\leftarrow\left[r(x)\right]^{-\frac{1}{2}}\exp\left[-\int_{x_2}^x r(t)dt\right]$$

(32)

and

$$\left[K(x)\right]^{-\frac{1}{2}}Cos\left[\int_x^{x_2}K(t)dt-\frac{\pi}{4}\right]\rightarrow\ -\left[r(x)\right]^{-\frac{1}{2}}\exp\left[\int_{x_2}^x r(t)dt\right].$$

(33)

4. SEMICLASSICAL QUANTIZATION CONDITION: BOHR-SOMMERFELD QUANTIZATION CONDITION.

A simple example of the application of the WKBJ approximation is presented here that served as a derivation of the lowest-order Bohr-Sommerfeld quantization rule [7, 13, 16, 27, 28]. The aim is to find the energy levels of a particle moving in the 0ne-dimensional potential well as shown in Fig. 1. For any assumed energy level E, there are just two turning points of the classical motion such that $V(x_1) = V(x_2) = E$. Consider equation (30) which is the connection formula at the classical turning point x_1 (*i.e.* the formula that connects the solution at the classically allowed region with the solution at the classically forbidden region), if

$$\Psi_1(x) = \alpha_1 [r(x)]^{-\frac{1}{2}} \exp[\int_x^{x_1} r(t)dt], \quad x < x_1 \quad (34)$$

this implies that

$$\Psi_2(x) = 2\alpha_2 [K(x)]^{-\frac{1}{2}} Cos\left[\int_{x_1}^x K(t)dt - \frac{\pi}{4}\right], \quad x_1 < x_2 \ (35)$$

and from equation (32) which is the connection formula at the classical turning point x_2, if

$$\Psi_3(x) = \alpha_3 [r(x)]^{-\frac{1}{2}} \exp[-\int_{x_2}^x r(t)dt], x_2 < x, \quad (36)$$

then

$$\Psi_4(x) = \alpha_4 [K(x)]^{-\frac{1}{2}} Cos[\int_x^{x_2} K(t)dt - \frac{\pi}{4}], x_1 < x_2. \quad (37)$$

Where $\alpha_i (i = 1, 2, 3, 4)$ are non-zero arbitrary constants.

Hence, in the interval $x_1 < x < x_2$ we have $\Psi_2(x) = \Psi_4(x)$.

Since $[K(x)]^{-\frac{1}{2}} \neq 0$,

$$\int_x^{x_2} K(t)dt = -\int_{x_1}^x K(t)dt + \int_{x_1}^{x_2} K(t)dt. \quad (38)$$

We can write that:

$$Cos\,[\int_{x}^{x_2} K(t)dt - \frac{\pi}{4}] = Cos\,\{[\int_{x_1}^{x} K(t)dt - \frac{\pi}{4}] - [\int_{x_1}^{x_2} K(t)dt - \frac{\pi}{2}]\}$$

$$= (-1)^n Cos[\int_{x_1}^{x} K(t)dt - \frac{\pi}{4}] \quad , \ (39)$$

provided

$$[\int_{x_1}^{x_2} K(t)dt - \frac{\pi}{2}] = n\pi \ ; n = 0,1,2,3... \ , \ (40)$$

which implies that

$$\alpha_4 Cos\,[\int_{x}^{x_2} K(t)dt - \frac{\pi}{4}] = (-1)^n \alpha_2 Cos[\int_{x_1}^{x} K(t)dt - \frac{\pi}{4}] \quad (41)$$

i.e.

$$\alpha_4 = (-1)^n \alpha_2 . \ (42)$$

Equations (40) and (42) are the conditions for which

$\Psi_2(x) = \Psi_4(x)$ in $x_1 < x < x_2$; in particular equation (40) is re-written

as :

$$\int_{x_1}^{x_2} \{2\mu\,[E - V(t)]\}^{\frac{1}{2}} dt = (n + \frac{1}{2})\hbar\pi \quad ; n = 0,1,2,3.. \quad (43)$$

or classically,

$$J = 2\pi(n + \frac{1}{2})\hbar = (n + \frac{1}{2})h , \, n = 0, 1, 2, 3, ... \quad (44)$$

Where

$$J = \oint P(t)dt = 2\int_{x1}^{x_2} P(t)dt . \quad (45)$$

Which is the required semiclassical quantization rule, which can be used to determine the allowed energy values E of a given potentials.

As earlier stated WKBJ approximation is a semiclassical approximation, since it is expected to be most useful in the nearly classical limit of large quantum numbers. The method will not be good for, say, the first few lowest states, so in order to overcome this shortcomings there is a need for a modified semiclassical quantization condition. For a particle oscillating between the two classical turning points x_1 and x_2, we obtain the semiclassical quantization condition by requiring that the total phase during one period of oscillation to be an integral multiple of 2π; [13] such that

$$\frac{J}{\hbar} - \phi_1 - \phi_2 = 2\pi n , \quad (46)$$

where ϕ_1 is the phase loss due to reflection at the classical turning point x_1 and ϕ_2 is the phase loss due to reflection at x_2. Equation (46) becomes

$$\frac{2}{\hbar}\int_{x_1}^{x_2} P(t)dt - \phi_1 - \phi_2 = 2\pi n. \quad (47)$$

Taking ϕ_1 and ϕ_2 to be equal to $\frac{\pi}{2}$ leads to the modified semiclassical quantization rule, i. e.

$$\int_{x_1}^{x_2} P(t)dt = (n+\frac{\tau}{4})\pi\,\hbar\;;\quad \tau = \frac{2\,(\phi_1+\phi_2)}{\pi}\,, \tag{48}$$

where τ is the Maslov index, which denotes the total phase loss during one period in units of $\frac{\pi}{2}$. It contains contributions from the phase losses ϕ_1 and ϕ_2 due to reflections at points x_1 and x_2, respectively. It is pertinent to note that taking $\phi_1 = \phi_2 = \frac{\pi}{2}$ and an integer Maslov index $\tau = 2$ in equation (48), we have the familiar semiclassical quantization rule i. e. equation (43).

2. 5. Conclusion

We have presented a method for the construction of WKBJ wavefunctions based on the explicit consideration of matching between the solutions obtained from classically allowed and classically inaccessible regions which involves a pure asymptotic approximation technique. The connection formulae derived are applied to obtain the Bohr-Sommerfeld quantization rule (Standard WKBJ quantization rule) and also, this quantization condition is extended to obtain the modified semiclassical quantization rule which involves phase losses at the classical turning points.

It is obvious that the modified semiclassical quantization rule will produce more accurate results than familiar (Standard) WKBJ quantization rule. To demonstrate the efficiency of this method, one

can apply this method to find the quantized energy of the Pöschl-Teller potential, Cornell potential and Wood-Saxon potential.

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