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WKBJ APPROACH TO QUANTUM-MECHANICAL TUNNELLING THROUGH A NON-RECTANGULAR POTENTIAL BARRIER

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ABSTRACT

At classical turning points the validity of the WKBJ methods is no more guaranteed and hence we implored the Kramers's connection formulae that connects the asymptotic solutions in classically allowed and classically forbidden (inaccessible) regions which are later applied to the transmission theory. The WKBJ method is applied to the problem of quantum-mechanical tunneling through a non-rectangular potential barrier (a special case of modified Pöschl-Teller potential barrier). Due to inaccurate results of WKBJ near the top of the barrier, we used Kemble's method that accounts for a quadratic behavior of the potential near the top of the barrier. In order to obtain the accuracy of the method we compare its results with the exact and Kemble's result for the potential. Although WKBJ approximation is expected to give better results for a potential of large amplitude.

INTRODUCTION

The WKBJ approximation is extensively used in the calculation of the tunneling coefficients for transmission through a potential barrier. The WKBJ method Merzbacher 1970 [1], Giler 1988 [2], Cocolicchio and Viggiano 1997 [3], has frequently been used to calculate the tunneling coefficient. The method was certainly known to farina 1976 [4] and may be traced back even earlier Froman and Froman 1965 [5]. In Quantum mechanics, asymptotic approximation is often used to calculate the tunneling coefficients for a one-dimensional potential barrier, which is important for applications in solid state physics, for example.

Tunneling coefficients calculations using WKBJ can be found in most Quantum mechanics textbooks for different potentials. Bohm 1952 [6], Landau and Lifshitz1977[7], Morse and Feshbach [8]. The validity of the JWKB formular for a triangular potential barrier was obtained by Ghatak et al 1977 [9]. The analytic expression for the tunneling coefficients is still of an instructive value for examples, tunneling and transition amplitude with the modified cubic potential, Martinez 1977 [10], Yanetka 1999 [11] obtained the transmission coefficients for the double delta-function potential embedded in a crystalline lattice. Although exact result serve as a comparison to obtain the accuracy of the WKBJ method. Modern computers now allow the tunnelling coefficients for a realistic potential to be calculated using WKBJ method with relative ease. Farina 1988 [12] obtained the transmission probability and traversal time in scattering by a one-dimensional potential of finite range. The tiny effect of the ground state energy in the case of a quantum mechanical potential with broken supersymmetry Giler et al 1986 [13].

The non-rectangular potential barrier (a special case of modified Pöschl-Teller potential) Ahmedov and Duru 1997 [14] , Grosche 1990 [15], Kleinert and Mustapic 1992 [16] which is a smooth potential has severally been studied by some researchers Chebotarev 1996 [17] Chebotarev 1997 [18], Chebotarev 1996 [19] as well and because of its known exact solutions of tunneling, Landau and Lifshitz 1977 [7].

The Kramers's connection formulae are as obtained in §2, WKBJ approximation method as applied to the transmission theory is contained in §3. In §4 we obtained the exact WKBJ and Kemble results for the tunneling coefficients for the non-rectangular potential. §5 contains results and discussions of results while we conclude with §6.

ASYMPTOTIC (OR WKBJ) APPROXIMATION METHOD

The wavefunction $\psi(x)$ that represents the particle's tunneling state in the potential V(x) satisfies the Schrodinger equation.

$$\frac{d^2\psi}{dx^2}+\frac{2\mu}{h^2}[E-v(x)]\psi(x)=0 \quad ,-\infty, x<\infty \tag{2.1}$$

We define

$$k(x)=\left\{\frac{2\mu}{h^2}[E-v(x)]\right\}^{1/2} \qquad if\ E\geq v(x)$$

$$=i\left\{\frac{2\mu}{h^2}[E-v(x)]\right\}^{1/2}$$

$$=ir(x);\ if\ E\leq v(x) \tag{2.2}$$

The semiclassical treatment of physical problems related to equation (2.1) is generally based on the theory of asymptotic representations for the solutions of equatio (2.1). as is known, in the domains where $k^2(x)$ may be considered to be large and slowly varying function, the conventional WKBJ approximation applies, which makes use of exponential functions for representing the solutions of equation (2.1) as the approximate wave function.

$$\psi(x)=\{k(x)\}^{1/2}\exp\left[\pm\int_{x_0}^{x}k(t)dt\right] \tag{2.3}$$

In the neighbourhoods of the turning points defined by $k^2(x)=0$, the WKBJ approximation fails. Since the condition for validity of equation (2.3) breaks down either at the classical turning points, where V(x)= E or anywhere V(x) has a steep gradient. This now follows that equation (2.3) becomes invalid around the classical turning points only, but Kramers's connection formulae gives the correct transfer of approximate solution from the non-classical region E < v(x) through a turning point to approximate solution valid in the classical region E > v(x), and vice-versa. Solutions about such points are derived by transforming the schrodinger equation to either airy or modified airy differential equations. The asymptotic expansion of these later solutions are appropriately connected (Kramers's connection formulae) with the WKBJ solutions to provide full range solutions as obtained by Morse and Feshbach 1953 [8]; Froman and froman, 1965 [5]; Giler, 1988 [2]; Cocolicchio and Viggiano, 1997 [3]; Oyewumi and bangudu, 1999 [20]. The two Kramers's connection formulae that are aplied to potential barrier penetration are the matching expression

$$[r(x)]^{-1/2} \exp\left[-\int_{x_1}^{x} r(t)dt\right] \rightarrow 2[k(x)]^{-1/2} Cos\left[\int_{x}^{x_1} k(t)dt - \frac{\pi}{4}\right] \tag{2.4}$$

And

$$[k(x)]^{-1/2} \sin\left[-\int_{x}^{x_2} k(t)dt - \frac{\pi}{4}\right] \rightarrow -2[r(x)]^{-1/2} \exp\left[\int_{x_2}^{x} r(t)\right] \tag{2.5}$$

WKBJ APPROXIMATION METHOD AS APPLIED TO PENETRATION OF POTENTIAL BARRIER

The WKBJ approximation method is now applied to potential barrier penetration upon which the particles are incidents from the left with insufficient energy to pass to the other side classically {E < $V(x)_{max}$ (Merzbacher, 1970 [1]; Farina, 1988 [12]; Cocolicchio amd Viggiano, 1997_[3]). If the approximation is assumed to hold in the three regions indicated in Fig 1 below:

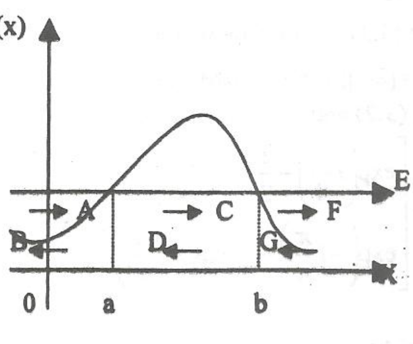

Fig 1: Transmission through a potential barrier

At the classical turning points V(a) = V(b) = E, some of the particles will pass onto the classically inaccessible region defined by E < V_{max}. from the solution of schrodinger equation (2.3), which can be written as follows:

For a < x;

$$\psi(x) = A[k(x)]^{-1/2} \exp\left[-i\int_x^a k(t)dt\right] + B[k(x)]^{-1/2} \exp\left[i\int_x^a k(t)dt\right] \qquad (3.1)$$

This can be rewritten as:

$$\psi(x) = \left[A\exp\left(-\frac{i\pi}{4}\right) + B\exp\left(\frac{i\pi}{4}\right)\right][k(x)]^{-\frac{1}{2}} Cos\phi + i\left[-A\exp\left(-\frac{i\pi}{4}\right)\right. \qquad (3.2)$$

$$\left. + B\exp\left(\frac{i\pi}{4}\right)\right][k(x)]^{-1/2} Sin\phi$$

Where $\phi = \int_x^a \left(K(t)dt - \frac{\pi}{4}\right)$ is called the phase integral.

3.2 for a < x< b;

$$\psi(x) = C[r(x)]^{-\frac{1}{2}} \exp\left[-\int_a^x r(t)dt\right] + D[r(x)]^{-\frac{1}{2}} \exp\left[\int_a^x r(t)dt\right] \qquad (3.3)$$

Using equations (2.4) and (2.5), we have that

$$[r(x)]^{-\frac{1}{2}} \exp\left[-\int_a^x r(t)dt\right] \to 2[k(x)]^{-\frac{1}{2}} Cos\left[\int_x^a k(t)dt - \frac{\pi}{4}\right] = 2[k(x)]^{-\frac{1}{2}} \cos\phi \qquad (3.4)$$

and

$$[r(x)]^{-\frac{1}{2}} \exp\left[-\int_a^x r(t)dt\right] \to -[k(x)]^{-\frac{1}{2}} Sin\left[\int_x^a k(t)dt - \frac{\pi}{4}\right] = -[k(x)]^{-\frac{1}{2}} Sin\phi \qquad (3.5)$$

Hence equation (3.3) can now be written as

$$\psi(x) = [2C][k(x)]^{-\frac{1}{2}} Cos\phi + [-D][k(x)]^{-\frac{1}{2}} Sin\phi \qquad (3.6)$$

With equations (3.2) and (3.6), we can relate their coefficients in matrix form as:

$$\begin{bmatrix} A \\ B \end{bmatrix} = \begin{bmatrix} \exp\left(i\frac{\pi}{4}\right) - \frac{i}{2}\exp\left(i\frac{\pi}{4}\right) \\ \exp\left(-i\frac{\pi}{4}\right) - \frac{i}{2}\exp\left(-i\frac{\pi}{4}\right) \end{bmatrix} \begin{bmatrix} C \\ D \end{bmatrix} \qquad (3.7)$$

3.3 For x < b;

We can write

$$\int_a^x r(t)dt = \theta - \int_x^b r(t)dt \qquad (3.8)$$

where $\theta = \exp\left[\int_a^b r(t)dt\right]$ (3.9)

So that equation (3.3) becomes

$$\psi(x) = \left[\frac{C}{\theta}\right][r(x)]^{-\frac{1}{2}} \exp\left[\int_x^b r(t)dt\right] + [D\theta][r(x)]^{-\frac{1}{2}} \exp\left[-\int_x^b r(t)dt\right] \quad (3.10)$$

3.4 For x > b;

$$\psi(x) = F[k(x)]^{-\frac{1}{2}} \exp\left[i\int_b^x k(t)dt\right] + G[k(x)]^{-\frac{1}{2}} \exp\left[-i\int_b^x k(t)dt\right] \quad (3.11)$$

This again can be rewritten as;

$$\psi(x) = \left[F\exp\left(i\frac{\pi}{4}\right) + G\exp\left(-\frac{i\pi}{4}\right)\right][k(x)]^{-\frac{1}{2}} Cos\,\alpha$$
$$+ i\left[F\exp\left(i\frac{\pi}{4}\right)\right] - G\exp\left(-\frac{i\pi}{4}\right)[k(x)]^{-\frac{1}{2}} \quad (3.12)$$

Where $\alpha = \int_b^x k(t)dt - \frac{\pi}{4}$

In the similar fashion of the usage of equations (2.4) and (2.5) in equation (3.10), the established relationships between the coefficients can now be written in the matrix form as:

$$\begin{bmatrix} C \\ D \end{bmatrix} = \begin{bmatrix} -i\theta\exp\left(i\frac{\pi}{4}\right) & i\theta\exp\left(i\frac{\pi}{4}\right) \\ \frac{1}{2\theta}\exp\left(i\frac{\pi}{4}\right) & \frac{1}{2\theta}\exp\left(-i\frac{\pi}{4}\right) \end{bmatrix} \begin{bmatrix} F \\ G \end{bmatrix} \quad (3.13)$$

Using the equation (3.7), we have;

$$\begin{bmatrix} A \\ B \end{bmatrix} = \frac{1}{2}\begin{bmatrix} \left(2\theta + \frac{1}{2\theta}\right) & i\left(2\theta - \frac{1}{2\theta}\right) \\ -i\left(2\theta - \frac{1}{2\theta}\right) & \left(2\theta + \frac{1}{2\theta}\right) \end{bmatrix} \begin{bmatrix} F \\ G \end{bmatrix} \quad (3.14)$$

θ measures the height and the width of the barrier (b – a) and is a function of energy. A particular solution of interest is obtained from equation (3.4) letting G = 0 (assuming no incident wave from the right). The transmission coefficient can now easily be calculated since

$$T = \frac{|j_{trans}|}{|j_{inc}|} = \frac{|F|^2}{|A|^2} \quad (3.15)$$

j is called the probability current density and hence:

$$T = \frac{4}{\left(2\theta + \frac{1}{2\theta}\right)^2} \qquad (3.16)$$

For a high and broad barrier (i.e. r(x) >> 0, (b – a) >> 0), we have θ >> 1 i.e. 1/θ << 1

$$T \approx \frac{1}{\theta^2} = \exp\left[-2\int_a^b r(t)dt\right] \qquad (3.17)$$

Therefore $T_{WKBJ} \approx \exp[-2Q]$ (3.18)

$$Q = \int_a^b r(t)dt$$

On the other hand the reflection coefficient R_{WKBJ} can be obtained as

$$R_{WKBJ} = 1 - T_{WKBJ} \qquad (3.19)$$

Asymptotic approximation is certainly the most usual method used for determining the penetrating factor of such a smooth potential barrier, a and b are the classical turning points corresponding to the actual value of the energy E. This approximation is only justified if the T_{WKBJ} is small. This is normally not the case near the top of the potential barrier, where Q tends to vanish. This reduces the validity of such an expression to a region of energy reasonably smaller than the maximum of the potential hill. Kemble, 1958 [21] has proposed a modification of the expression accounting for a quadratic behaviour of the potential near the top of the barrier.

The expression (also quoted by Chebotarev, 1996[19])

$$T_{kemble} = \frac{1}{1+\exp[2Q]} \qquad (3.20)$$

and the corresponding

$$R_{kemble} = \frac{1}{1+\exp[-2Q]} \qquad (3.21)$$

being exact for a parabolic hill and identical to equation (3.18) and (3.19) for large Q.

THE EXACT SOLUTION, WKBJ AND KEMBLE APPROACHES FOR THE TUNNELLING, COEFFICIENTS FOR THE NON-RECTANGULAR POTENTIAL BARRIER

The reflection and transmission coefficients produced by WKBJ approximation method as obtained in section 3 is now compared with the exact and the Kemble mode of approximation results. The case been comsidered is the well-known model: A special case of modified Poschl-Teller potential (i.e. a non-rectangular potential barrier). Ahmedov and Duru 1997 [14], grosche 1990 [15]; Kleinert and Mustapic 1992 [15].

$$V(x) = \frac{\lambda^2 + 1/4}{Cosh^2 x} \quad ,\lambda > 0 \qquad (4.1)$$

For the reason that the exact solution of thre tunnelling problem V(x) = 1/Cosh^{2}x is known, as obtained by Landau and Liftshits 1977 [7], and also several works has been done with this potential by Chebotarev 1996 [17], Chebotarev 1997 [18], Chebotarev 1996 [19]. Equation (4.1) can be treated exactly at least for energies E smaller than the maximum potential value $E < \lambda^2 + ¼$. The exact reflection and transmission coefficients are given by:

$$R_{Exact} = \frac{Cos^2\left[\frac{\pi}{2}\sqrt{1-(4\lambda^2+1)}\right]}{Sinh^2(\pi\sqrt{E}) + Cos^2\left[\frac{\pi}{2}\sqrt{1-(4\lambda^2+1)}\right]} \qquad (4.2)$$

$$T_{Exact} = \frac{Sinh^2\left[\pi\sqrt{E}\right]}{Sinh^2(\pi\sqrt{E}) + Cos^2\left[\frac{\pi}{2}\sqrt{1-(4\lambda^2+1)}\right]} \qquad (4.3)$$

From equations (3.18) and (4.1) we have

$$Q = \int_a^b \left[\frac{\lambda^2 + \frac{1}{4}}{Cosh^2 x} - E\right]^{\frac{1}{2}} dx \qquad (4.4)$$

We put J(E) = Q to evaluate integral (4.4) and on differentiating both sides with respect to E as far as the differentiation of the upper and lower limits of the integrals is concerned that which depends on E vanishes since the expression under the square root is equal to zero at the turning points i.e.

$$J'(E) = -\frac{1}{2}\int_a^b \left[\frac{\lambda^2 + \frac{1}{4}}{Cosh^2 x} - E\right]^{-\frac{1}{2}} dx \qquad (4.5)$$

Where a and b are the solutions of $\frac{\lambda^2 + \frac{1}{4}}{Cosh^2 x} - E = 0$ and putting y = sinh x,

$$J'(E) = -\frac{1}{2}\int_{y_1}^{y_2} \frac{dy}{[(\lambda^2 + \frac{1}{4}) - E(1+y^2)]^{\frac{1}{2}}} \qquad (4.6)$$

Where y_1 and y_2 are the solutions of $\frac{\lambda^2 + \frac{1}{4}}{1+y^2} - E = 0$

Putting $Sin\theta = \left\{\frac{E}{[(\lambda^2 + \frac{1}{4}) - E]}\right\}^{\frac{1}{2}} y$ in equation (4.6), we have

$$J'(E) = -\frac{1}{2\sqrt{E}}\left[\theta_2 - \theta_1\right] \qquad (4.7)$$

Where θ_1 and θ_2 are solutions of $\dfrac{\lambda^2 + 1/4}{1 + \dfrac{[(\lambda^2 + 1/4) - E]Sin^2\theta}{E}} - E = 0$

i.e.

$$E\left[\left(\lambda^2 + \frac{1}{4}\right) - E\right]Sin^2\theta = E\left[\left(\lambda^2 + \frac{1}{4}\right) - E\right]$$

Then, $Sin^2\theta = 1$, which implies that $\theta_2 = \frac{\pi}{2}, \theta_2 = -\frac{\pi}{2}$

Then, $J'(E) = -\dfrac{\pi}{2E}$

$$J(E) = -\pi\sqrt{E} + C_1 \qquad (4.8)$$

The constant C_1 can be determined by observing that $E = \lambda^2 + 1/4$ the range of integration reduces to the point $x = 0$.

a and b are the solutions of $\dfrac{\lambda^2 + 1/4}{Cosh^2 x} - \left(\lambda^2 + \dfrac{1}{4}\right) = 0$

implies that $Cosh\, x = \pm 1$ i.e. $x = 0 \Rightarrow a = b = 0$.

i.e. $J\left(\lambda^2 + \dfrac{1}{4}\right) = -\pi\sqrt{\left(\lambda^2 + \dfrac{1}{4}\right)} + C_1 = 0$

$$C_1 = -\pi\sqrt{\left(\lambda^2 + \frac{1}{4}\right)}$$

Therefore,

$$Q = J(E) = \pi\left[\sqrt{\left(\lambda^2 + \frac{1}{4}\right)}\right] - \sqrt{E} \qquad (4.9)$$

5 RESULTS AND DISCUSSION

For the case $\lambda^2 = \dfrac{3}{4}$ then $V(x) = \dfrac{1}{Cosh^2 x}$ (5.1)

Then the energy of the particles $E < 1$.

Table 1: Comparison between the exact, WKBJ and Kemble approaches for the determination of the reflection coefficient for the potential $1/Cosh^2x$

Energy	Exact (4.2)	WKBJ (3.19)	Kemble (3.21)
0.10	9.772033655 E-01	9.863807040E-01	9.865636970E-01
0.20	9.407168359E-1	9.689842280E-1	9.699172670E-1
0.30	8:883194078E-01	9.416760801E-01	9.448902950E-01
0.40	8.196785640E-01	9.006742080E-01	9.096484480E-01
0.50	7.370761318E-01	8.412305890E-01	8.629844640E-01
0.60	6.453279771E-01	7.573780078E-01	8.047500002E-01
0.70	5.507264927E-01	6.416679910E-01	7.361970360E-01
0.80	4.594537186E-01	4.848687333E-01	6.600088020E-01
0.90	3.762386597E-01	2.756150640E-01	5.799169190E-01
1.00	3.037717995E-01	0.000000000E-01	5.000000000E-01

Table 2: Comparison between the exact, WKBJ and Kemble approaches for the determination of the transmission coefficient for the potential $1/Cosh^2x$

Energy	Exact (4.2)	WKBJ (3.19)	Kemble (3.21)
0.10	2.279663450 E-02	1.361929600E-01	1.343630300E-01
0.20	5.928316410E-02	3.101577200E-1	3.008273300E-1
0.30	1.116805922E-01	5.832391900E-01	5.510970500E-01
0.40	1.803214360E-01	9.932579200E-01	9.035155200E-01
0.50	2.629238682E-01	1.587694110E-01	1.370155350E-01
0.60	3.546720229E-01	2.426219280E-01	1.952499970E-01
0.70	4.492735073E-01	3.583320090E-01	2.638029630E-01
0.80	5.405462814E-01	5.151312670E-01	3.399911800E-01
0.90	6.237613403E-01	7.243849360E-01	4.200830800E-01
1.00	6.962282005E-01	1.000000000	5.000000000E-01

For the case $\lambda^2 = \frac{1319}{100}$, then $V(x) = \frac{13.44}{Cosh^2 x}$ (5.2)

The energy of the particle in this case is $E < 13.44$.

Table 3 Comparison between the exact, WKBJ and Kemble approaches for the determination of the reflection coefficient for the potential $13.44/\text{Cosh}^2 x$

Energy	Exact (4.2)	WKBJ (3.19)	Kemble (3.21)
1.68	9.999995770E-01	9.999996587E-01	9.999996587E-01
3.36	9.999876525E-1	9.999898671E-1	9.999900434E-1
5.04	9.998356886E-01	9.998674859E-01	9.998675035E-01
6.72	9.985451834E-01	9.988252030E-01	9.988265815E-01
8.40	9.901354694E-01	9.919665141E-01	9.920305366E-01
10.08	9.463840754E-01	9.543176333E-01	9.563133431E-01
11.76	7.811635909E-01	7.741085430E-01	8.157329054E-01
13.44	4.463966514E-01	0.000000000	5.000000000E-01

Table 4 Comparison between the exact, WKBJ and Kemble approaches for the determination of the transmission coefficient for the potential $13.44/\text{Cosh}^2 x$

Energy	Exact (4.2)	WKBJ (3.19)	Kemble (3.21)
1.68	4.229804745E-07	3.412676148E-07	3.416674983E-07
3.36	1.234745450E-05	1.013293042E-05	1.004362892E-05
5.04	1.643114135E-04	1.325140620E-04	1.324965040E-04
6.72	1.454816601E-03	1.174796945E-03	1.173418455E-03
8.40	9.864530600E-03	8.033485945E-03	7.969463373E-03
10.08	5.361592440E-02	4.568236675E-02	4.368665687E-02
11.76	2.188364091E-01	2.258914570E-01	1.842670946E-01
13.44	5.536033486E-01	1.000000000	5.000000000E-01

Kemble's method does not provide a better result than the WKBJ method except perhaps near $E \approx 1$, (for equation 5.1) where both give quite inaccurate results as in table 1 and 2.

Although as expected when the height of the potential barrier is made higher by multiplying the previous potential by some large amplitude of factor 336/25, the WKBJ provides a better approximation.

Table 3 and 4 compare the semiclassical approximation method with the exact method and kemble mode of approximation. However, for energies lying near the top of the barrier, the WKBJ approach becomes less accurate although Kemble's method becomes useful at that level since Kemble's method accounts for a quadratic behaviour of the potential barrier near the top of the barrier.

6 CONCLUSON

The semiclassical approximation method proposed here to evaluate the reflection and transmission coefficients of a non-rectangular potential barrier (a special case of modified Poschl-Teller potential barrier) is based on the applications of the Kramers's connection formulae (i.e. valid around the classical turning points) to the tunneling coefficients.

The method retains its most important features i.e. the sufficient condition for the semiclassical treatment to be valid in tunnelling problems is given by $E < \lambda^2 + \frac{1}{4}$, although the critical points are the base of the barrier $E = 0$ and the top of the barrier that $E = \lambda^2 + \frac{1}{4}$ where quite inaccurate results are obtained for the WKBJ method. Since the exact expressions for the tunneling coefficients for the non-rectangular potential barrier equation 4.1 are known, Laudau and Lifshitz 1977 [7] the results obtained within the semiclassical approximation method may be compared with the exact ones.

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