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DISCRETE EIGENVALUES OF A MODIFIED PÖSCHL – TELLER POTENTIAL HOLE USING SEMI-CLASSICAL APPROXIMATION

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ABSTRACT

The use of a modified Pöschl-Teller potential hole is addressed using both semi-classical path integral and Exact methods. The exact results of eigenvalues of a modified Pöschl-Teller potential hole is obtained on solving the one-dimensional Schrödinger equation for this potential hole analytically, which shows the accuracy of the semi-classical method. The approximate quantization rules (the well known Bohr-Sommerfeld quantization conditions) are derived from the W.K.B.J. formulae (solutions). The semi-classical method is then tested by the quantization of the quantum mechanical systems of the modified Pöschl-Teller potential hole which practically gives the same results as using exact method.

1. INTRODUCTION

The W.K.B.J. formula (Wentzel 1926, Kramers, 1926, Brilliouin 1926 and Jeffreys 1923) [1], [2] Cocolicchio & Viggiano, 1997 [3] provides us with rather simple and interestingly good approximate solution to the Schrödinger equation, for this reason it is widely used in many approximate calculations of quantum mechanical systems. Different tunnelling effects, as well as other effects caused by potential barriers Giler et al 1986 [4], Farina 1988 [5], Méndez and Dominguez-Adame 1994 [6] are examples in which the use of the W.K.B.J. formulae give correct results.

Other forms of the applications of this approximation method is the well known Bohr-Sommerfeld quantization conditions. For examples, Oyewumi and Bangudu 1998 [7] used W.K.B.J. method with the derivation of Bohr-Sommerfeld quantization conditions, obtained the discrete eigenvalues (quartic) oscillator which agrees with Giler's result of 1988 [1]. Giler used kth generalised Bohr-Sommerfeld quantization conditions, Ghatak et al 1997 [8] applied the JWKB formula to a triangular potential barrier and compare the resits with the exact results, also Birx and Hourk 1977 [9] obtained the eigenvalues for the upper and lower bounds of anharmonic oscillator potential. Although WKB fails to predict the individual energy levels (and also their wavefuncitons) within a vanishing fraction of mean energy level spacing in the limit when the quantum number goes to infinity Robnik and Salasnich 1997 [10].

The exact results of eigenvalues of a modified Pöschl-Teller potential hole is as obtained in §2 on solving the one-dimensional Schrödinger equation for this potential hole analytically. While §3 contains the derivation of Bohr-Sommerfeld quantization conditions through W.K.B.J. formulae. The application of this semi-classical approximation method to modified Pöschl-Teller potential hole and the comparison of the results of the exact method with the semi-classical method is contained in §4. While §5 contains discussion of results and we conclude with §6.

2. EXACT EIGENVALUES OF A MODIFIED PÖSCHL-TELLER POTENTIAL HOLE

The non-trivial potential, modified Pöschl-Teller potential hole for which the exact solution of the discrete energy is known is used in which the semi-classical approximation method gives an accurate results. Chebotarev 1996 [11] obtained the total delay time and tunnelling time for non-rectangular potential barriers and used modified Pöschl-Teller potential hole as an example which its exact result is known. Grypeos and Liolios 1997 [12] used the Hypervirial theorems (HVT) in conjunction with the Hellman-Feynman theorem (HFT) which provide a very powerful scheme for the treatment of the Even-Power potentials and one of the examples used is modified Pöschl-Teller potential hole and with the method its energy compared favourably with the exact analytic expression. Infact this potential also has been used rather extensively in studieis of hypernuclei, Lalazissis et al 1988 [13], Lalazissis 1994 [14] and Lalazissis 1993 [15].

An interesting feature of this potential is that the corresponding Schrödinger eigenvalue problem can be solved exactly.

The modified Pöschl-Teller potential hole [8] & [9] is given by

$$V(x) = \frac{-\hbar^2 \alpha^2 \lambda(\lambda - 1)}{2\mu \operatorname{Cosh}^2 \alpha x} \tag{2.1}$$

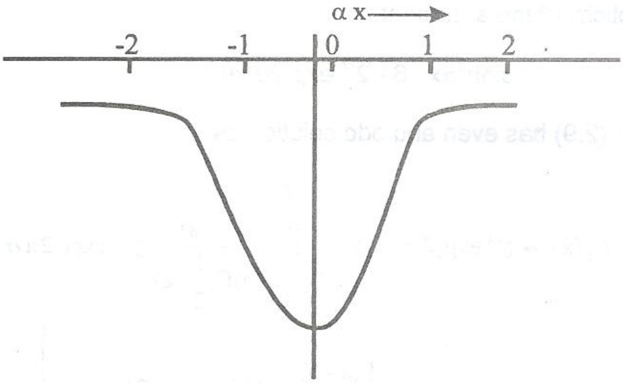
With $\lambda > 1$

The one-dimensional Schrödinger equation for the modified Pöschl-Teller potential hole is:

$$\Psi''(x) + \left[k^2 + \frac{\alpha\lambda(\lambda - 1)}{\operatorname{Cosh}^2 \alpha x}\right]\Psi(x) = 0 \tag{2.2}$$

$$\text{with } k^2 = \frac{2\mu}{\hbar^2} \tag{2.3}$$

Fig. 1: Modified Pöschl-Teller Potential Hole



We introduce the new variable;

$$y = \text{Cosh}^2 \alpha x \tag{2.4}$$

We obtain

$$y(1-y)\Psi''(y) + \left[\frac{1}{2} - y\right]\Psi'(y) - \left[\frac{k^2}{4\alpha^2} + \lambda(\lambda-1)\right]\Psi(y) = 0 \tag{2.5}$$

On substituting,

$$\Psi(y) = y^{\lambda/2}\, U(y) \tag{2.6}$$

To split off a fitting power of y, we arrive at the hypergeometric differential equation [18]

$$y(1-y)\,U''(y) + \left[\left(\lambda + \frac{1}{2}\right) - (\lambda+1)\,y\right]U'(y) - \frac{1}{4}\left(\lambda^2 + \frac{k^2}{\alpha^2}\right)U(y) = 0 \tag{2.7}$$

$$a = \frac{1}{2}\left(\lambda + \frac{ik}{\alpha}\right);\ b = \frac{1}{2}\left(\lambda - \frac{ik}{\alpha}\right) \tag{2.8}$$

The complete solution of equation (2.7) may be written as:

$$U(x) = AF(a, b, \frac{1}{2}; 1-y) + B(1-y)^{1/2} F\left(a+\frac{1}{2}, b+\frac{1}{2}, \frac{3}{2}; 1-y\right) \qquad (2.9)$$

This can be simplified further using [1] with the boundary conditions and the asymptoticity of the argument,

$$-\sinh^2\alpha x \quad 6 - 2^{-2}\exp(2\alpha|x|)$$

Equation (2.9) has even and odd solution as:

$$\Psi_e(x) \to 2^{-\lambda}\exp(\lambda\alpha|x|)\Gamma\left(\frac{1}{2}\right)\left\{\frac{\Gamma(b-a)}{\Gamma(b)\Gamma(\frac{1}{2}-a)}2^{2a}\exp(-2a\alpha|x|)\right.$$

$$\left. + \frac{\Gamma(a-b)}{\Gamma(a)\Gamma(\frac{1}{2}-b)}2^{2b}x\exp(-2b\alpha|x|)\right\} \qquad (2.10a)$$

$$\Psi_o(x) \to \pm 2^{-(\lambda+1)}\exp[(\lambda+1)\alpha|x|]\Gamma\left(\frac{3}{2}\right)\left\{\frac{\Gamma(b-a)}{\Gamma(b+\frac{1}{2})\Gamma(1-a)}2^{2a+1}\exp(-(2a+1)\alpha|x|]\right.$$

$$\left. + \frac{\Gamma(a-b)}{\Gamma\left(a+\frac{1}{2}\right)\Gamma(1-b)}2^{2b+1}\exp[-(2b+1)\alpha|x|]\right\} \qquad (2.10b)$$

Then , equation (2.2) now, compose a linear combination of the two fundamental solutions:

$$\psi(x) = A\psi_e(x) + B\psi_o(x)$$

We express

$$\psi_e \to C_e \operatorname{Cos}(k|x| + \phi_e); \; \psi_o \to \pm C_o \operatorname{Cos}(k|x| + \phi_o)$$

where,

$$\phi_e = \arg \frac{\Gamma\left(i\frac{k}{\alpha}\right)\exp\left(-i\frac{k}{\alpha}\log 2\right)}{\Gamma\left(\frac{\lambda}{2}+i\frac{k}{2\alpha}\right)\Gamma\left(\frac{1-\lambda}{2}+i\frac{k}{2\alpha}\right)} \tag{2.11}$$

and

$$\phi_o = \arg \frac{\Gamma\left(i\frac{k}{\alpha}\right)\exp\left(-i\frac{k}{\alpha}\log 2\right)}{\Gamma\left(\frac{\lambda+1}{2}+i\frac{k}{2\alpha}\right)\Gamma\left(1-\frac{\lambda}{2}+i\frac{k}{2\alpha}\right)} \tag{2.12}$$

From equation (2.3), we have

$$E = \frac{\hbar^2 K^2}{2\mu}$$

and for bound state E < 0. (i.e. Eigenvalues exist for negative energies, we put k = iχ

$$\text{i.e. } E = \frac{-\hbar\chi^2}{2\mu} \tag{2.13}$$

and the parameters in equation (2.8) become real, viz:

$$a = \frac{1}{2}\left(\lambda - \frac{\chi}{\alpha}\right); b = \frac{1}{2}\left(\lambda + \frac{\chi}{\alpha}\right) \tag{2.14}$$

We may again use the asymptotic formulae (2.10a) and (2.10b) in which, however the first term now behaves as exp (α|x|) and the second as exp (-α|x|).

A normalizable solution is therefore possible for χ > 0, if and only If, the factor of the first term vanishes. Since the Γ functions are now all taken for real arguments where poles exist at negative integers, - n (n = 0, 1, 2, 3...) The eigenvalues follow from:

$$\frac{1-\lambda}{2} + \frac{\chi}{2\alpha} = -n \text{ or } \frac{\chi}{\alpha} = \lambda - 1 - 2n \tag{2.15}$$

for even eigenstates.
and

$$1 - \frac{\lambda}{2} + \frac{\chi}{2\alpha} = -n \text{ or } \frac{\chi}{\alpha} = \lambda - 2 - 2n \qquad 2.16$$

for odd eigenstates
Hence, the eigenstates (energy terms) become, with a slight change in notations (for even and odd eigenstates)

$$En = -\frac{{}^2\alpha^2}{2\mu}(\lambda - 1 - n)^2, n = 0,1,2,3 \qquad 2.17$$

3.0 ENERGY LEVELS OF A POTENTIAL WELL (BOHR-SOMERFELD QUANTIZATION RULE)

In the semi-classical approximation the determination of discrete energy levels in the potential well V = V(x) reduces to finding the conditions under which real exponential W.K.B.J. solution vanish asymptotically in regions I and III [2]. Thus in region I, we have,

$$\Psi_1(x) = \alpha_1 [r(x)]^{-\frac{1}{2}} \exp\left(-\int_x^a r(t)\,dt\right), \quad x < a \qquad (3.1)$$

Implies that

$$\Psi_2(x) = \alpha_2 . 2[k(x)]^{-\frac{1}{2}} \operatorname{Cos}\left(\int_a^x k(t)\,dt - \frac{\pi}{4}\right), \quad a < x < b \qquad (3.2)$$

And in region III, if,

$$\Psi_3(x) = \alpha_3 2[r(x)]^{-\frac{1}{2}} \exp\left(-\int_a^x r(t)\,dt\right), x < b \qquad (3.3)$$

Then

$$\Psi_4(x) = \alpha_4 . 2[k(x)]^{-\frac{1}{2}} \operatorname{Cos}\left(\int_x^b k(t)\,dt - \frac{\pi}{4}\right), \quad a < x < b \qquad (3.4)$$

where

σ_i (I = 1, 2, 3, 4) are non-zero arbitrary constants

where k(x) is defined as:

$$k(x) = \left\{\frac{2\mu}{\hbar^2}[E - v(x)]\right\}^{\frac{1}{2}}, \text{ If } E > v(x)$$

As earlier been stated W.K.B.J. method is a semi-classical approximation, since it is expected to be most useful in the nearly classical limit of large quantum numbers. Equation (3.13) can be used to determine the discrete eigenvalues of any given potential.

4. EIGENVALUES OF A MODIFIED PÖSCHL-TELLER POTENTIAL HOLE USING SEMI-CLASSICAL APPROXIMATION

The energy levels of this potential in semi-classical approximation are obtained from condition (3.13). Where V(x) is as given in equation (2.1); a and b are now the solution of the equation (4.1)

To evaluate the integral

$$J(E)=\int_a^b\left[\frac{2\mu}{\hbar^2}\left\{E+\frac{\hbar^2\alpha^2\lambda(\lambda-1)}{2\mu\cosh^2\alpha x}\right\}\right]^{\frac{1}{2}}dx \tag{4.2}$$

We should note that for bound state En < 0 for the case under consideration of a discrete spectrum.

On differentiating equation (4.2) with respect to E, the upper and the lower limits of the integral as far as the differentiation is concerned that which depends on E vanishes since the expression under the square root is equal to zero at the turning points a and b. We get thus:

$$J^1(E)=\frac{\mu}{\hbar^2}\int_a^b\left\{\frac{2\mu}{\hbar^2}\left[E+\frac{\hbar^2\alpha^2\lambda(\lambda-1)}{2\mu\cosh^2\alpha x}\right]\right\}^{-\frac{1}{2}}dx \tag{4.3}$$

where a & b are solutions of

$$E+\frac{\hbar\alpha^2\lambda(\lambda-1)}{2\mu\,\mathrm{Cosh}^2\alpha x}=0 \tag{4.4}$$

Putting

$$\eta=\mathrm{Sinh}\alpha x \tag{4.5}$$

Equation (4.3) becomes

$$J'(E)=\frac{\mu}{\alpha\hbar}\int_{\eta_1}^{\eta_2}\frac{d\eta}{\left[2\mu E(1-\eta^2)+\alpha_0\right]^{\frac{1}{2}}} \tag{4.6}$$

where $\alpha_o = \dfrac{\hbar^2\alpha^2\lambda(\lambda-1)}{2\mu}$ (4.7)

$$J'(E) = \frac{\mu}{\alpha\hbar\left[2\mu(E+\alpha_0)\right]^{1/2}} \int_{\eta_1}^{\eta_2} \frac{d\eta}{\left[1 + \frac{E}{E+\alpha_0}\cdot\eta^2\right]^{\frac{1}{2}}} \quad (4.8)$$

Where η_2 and η_1 are the solutions of (as from equation 4.4)

$$E + \frac{\alpha_o}{1+\eta^2} = 0 \quad (4.9)$$

Now, putting $\eta = [(E + \alpha_o)/E]^{1/2} \sin h\,\theta$ (4.10)
then, equation (4.8) becomes,

$$J'(E) = \frac{\mu}{\alpha\hbar[2\mu E]^{\frac{1}{2}}}[\theta_2 - \theta_1] \quad (4.11)$$

where θ_1 and θ_2 are the solutions of:

$$E + \left[\frac{\alpha_o}{1 + \frac{E+\alpha_o}{E}\text{Sin h}^2\theta}\right] = 0 \quad (4.12)$$

i.e. $E(E + \sigma_o) \sin h^2\,\theta = -(E^2 + E\sigma_o)$ (4.13)

$$\theta_1 = -i\frac{\pi}{2}; \theta_2 = i\frac{\pi}{2} \quad (4.14)$$

Therefore, $J'(E) = \dfrac{\mu\pi}{\alpha\hbar(-2\mu E)^{1/2}}$ (4.15)

$$J(E) = -\frac{\pi}{\alpha\hbar}(-2\mu E)^{1/2} + c_1 \quad (4.16)$$

The constant of integration, C_1 can be determined by observing that for $E = -\alpha_o$, the range of integration in equation (4.2) reduces to the point x = 0.
i.e. a and b are solutions of

$$= i\left\{\frac{2\mu}{\hbar^2}\left[v(x) - E\right]\right\}^{\frac{1}{2}} = ir(x), \text{ If } E < v(x) \tag{3.5}$$

As in Figure II, there are supposed to be just two turning points of the classical motion such that,

$\psi_2(x) = \psi_4(x)$, in the interval $a < x < b$.

$$\text{i.e. } \alpha_2 \cos\left(\int_a^x k(t)\,dt - \frac{\pi}{4}\right) = \alpha_4 \operatorname{Cost}\left(\int_x^b k(t)\,dt - \frac{\pi}{4}\right) \tag{3.6}$$

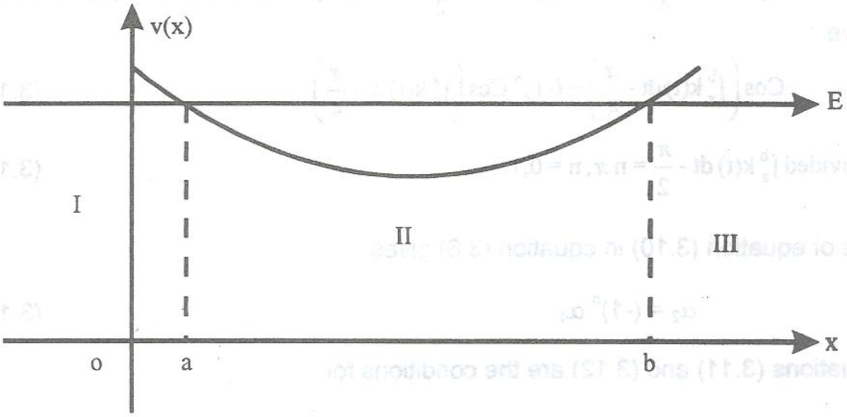


Fig. II: Application of the W.K.B.J. Method to a potential trough: Linear turning points occur at a and b.

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

The fact that $\int_x^b k(t)\,dt = \int_x^a k(t)\,dt + \int_a^b k(t)\,dt$

$$= -\int_a^x k(t)\,dt + \int_a^b k(t)\,dt \tag{3.7}$$

And $\cos(-\theta) = \cos\theta$ (is an even function of θ)
Then,

$$\mathrm{Cos}\left(\int_x^b k(t)\,dt - \frac{\pi}{4}\right) = \cos\left[-\int_a^x k(t)\,dt + \int_a^b k(t)\,dt - \frac{\pi}{4}\right] \tag{3.8}$$

$$= Cos\left[\left(\int_a^x k(t)\,dt - \frac{\pi}{4}\right) - \left(\int_a^b k(t)\,dt - \frac{\pi}{2}\right)\right] \tag{3.9}$$

Since Cos ($-\theta$) = Cosθ

and also from Trigonometrical property,

Cos (A -B) = CosA CosB + SinA SinB

= $(-1)^n$ CosA, Provide B = nπ; n = 0, 1, 2, ...

with $A = \int_a^x k(t)\,dt - \frac{\pi}{4}$, and $B = \int_a^b k(t)\,dt - \frac{\pi}{2}$. In the right hand side of equation (3.9) we have:

$$\mathrm{Cos}\left(\int_x^b k(t)\,dt - \frac{\pi}{4}\right) = (-1)^n\,\mathrm{Cos}\left(\int_a^x k(t)\,dt - \frac{\pi}{4}\right) \tag{3.10}$$

$$\text{Provided} \int_a^b k(t)\,dt - \frac{\pi}{2} = n\,\pi, n = 0,1,2,... \tag{3.11}$$

use of equation (3.10) in equation (3.6) gives

$$\alpha_2 = (-1)^n\,\alpha_4 \tag{3.12}$$

equations (3.11) and (3.12) are the conditions for

$\psi_2(x) = \psi_4(x)$, in the interval $a < x < b$.

In particular, equation (3.11) can be written as

$$\int_a^b k(t)\,dt = (n + \frac{1}{2})\pi, n = 0,1,2,3...$$

or, by virtue of equation (3.5a) as:

$$\int_a^b \left[\frac{2\mu}{\hbar^2}(E - v(t))\right]^{\frac{1}{2}} dt = \left(n + \frac{1}{2}\right)\pi, n = 0,1,2,3... \tag{3.13}$$

is the required Both-Sommerfeld quantization rule.

$$-\alpha_o + \frac{\alpha_o}{\text{Cosh}^2 \alpha x} = 0$$

This implies that J-α_o) = 0

Then, $C_1 = \frac{\pi(2\mu\alpha_o)^{\frac{1}{2}}}{\alpha\hbar}$

Condition (3.13) now gives

$$(-2\mu\bar{E}_n)^{1/2} = (2\mu\alpha_o)^{1/2} - \alpha\hbar\left(n + \frac{1}{2}\right)$$

Therefore,

$$\bar{E}_n = -\frac{\alpha^2\hbar^2}{2\mu}\left[\left(\frac{2\mu\alpha_o}{\alpha^2\hbar^2}\right)^{\frac{1}{2}} - \left(n + \frac{1}{2}\right)\right]^2, n = 0,1,2,3,... \qquad (4.18)$$

The discrete energy levels for a modified Pöschl-Teller potential hole is,

$$\bar{E}_n = -\frac{\alpha^2\hbar^2}{2\mu}\left\{[\lambda(\lambda -)]^{\frac{1}{2}} - \left(n + \frac{1}{2}\right)\right\}^2, n = 0,1,2,3,... \qquad (4.19)$$

The exact eigenvalues E_n of the modified Pöschl-Teller potential hole is as obtained in equation (2.17) and that using semi-classical approximation $\bar{E}_n$ is as obtained in equation (4.19).

If we let $\hbar^2\alpha^2 = 2\mu$ in the two cases, then, we have

$$E_n = -(\lambda - 1 - n)^2, n = 0, 1, 2, \qquad (4.20)$$

and

$$\bar{E}_n = \left\{[\lambda(\lambda - 1)]^{\frac{1}{2}} - n - \frac{1}{2}\right\}^2, n = 0,1,2,.. \qquad (4.21)$$

We obtain the values of E_n and $\bar{E}_n$ for integer and non-integer λ (odd and even also), where $|\epsilon| = |E_n - \bar{E}_n|$

The discrete energy levels for a modified Pöschl-Teller potential hole is

Table 1: The Values of E_n $\overline{E}_{n'}$ and $|\epsilon|$ with different values of λ.

n	$\lambda = 1.5$			$\lambda = 2$			$\lambda = 5$			$\lambda = 10$		
	E_n	$\overline{E}_{n'}$	$\|\epsilon\|$	E_n	$\overline{E}_{n'}$	$\|\epsilon\|$	E_n	$\overline{E}_{n'}$	$\|\epsilon\|$	E_n	$\overline{E}_{n'}$	$\|\epsilon\|$
0	- 0.250	- 0.137	0.113	-1.000	-0.836	0.164	-16.000	-15.778	0.222	-81.000	-80.763	0.237
1	- 0.250	- 0.397	0.147	0.000	-0.007	0.007	-9.000	-8.834	0.166	-64.000	-63.790	0.210
2	- 2.250	- 2.657	0.407	-1.000	-1.179	0.179	-4.00	-3.889	0.111	-49.000	-48.816	0.184
3	- 6.250	- 6.917	0.667	-4.000	-4.351	0.351	-1.000	-0.945	0.055	-36.000	-35.842	0.158
4	-12.250	- 13.177	0.927	-9.000	-9.522	0.522	0.000	-0.001	0.001	-25.000	-24.869	0.131
5	-20.250	- 21.437	1.187	-16.000	-16.694	0.694	-1.000	-1.057	0.057	-16.000	-15.895	0.105
6	-30.250	- 31.697	1.447	-25.000	-25.865	0.865	-4.000	-4.112	0.112	-9.000	-8.921	0.079
7	-42.250	- 43.957	1.707	-36.000	-37.037	1.037	-9.000	-9.168	0.168	-4.000	-3.946	0.054
8	-56.250	- 58.217	1.967	-49.000	-50.208	1.208	-16.000	-16.224	0.224	-1.000	-0.974	0.026
9	-72.250	- 74.447	2.227	-64.000	-65.380	1.380	-25.000	-25.279	0.279	0.000	0.000	0.000
10	-90.250	- 92.737	2.487	-81.000	-82.552	1.552	-36.000	-36.335	0.335	-1.000	-1.027	0.027

5. DISCUSSION OF RESULTS.

The even and odd eigenstates as in equations (2.15) and (2.16) can be combined as one as in equation (2.17) i.e. $E_n = -\frac{\hbar^2\alpha^2}{2\mu}(\lambda - 1 - n)^2, n = 0,,2,...$ which is identical with equation (4.19), Hence the semi-classical approximation method gives nearly the exact energy levels for the modified Pöschl-Teller potential hole.

Table I shows that the eigenvalues are less than zero. For the exact results (E_n), it is noted that for integer λ there is always one eigenvalue ($n = \lambda - 1$) lying at zero energy while on the other hand, semi-classical approximation method nearly (asymptotically) lying at zero energy.

$|\in|$ is the modulus of the difference between the corresponding values of n for E_n and $\overline{E_n}$.

For non-integer λ (λ = 1:5), $|\in|$increases as n increases, likewise λ = 2, λ = 5 but for λ = 10 the maximum value of $|\in|$= 0.237 occurs when n = 0 and decreases with increasing n to $|\in|$ = 0.027 (when n = 10), This indirectly confirms the description of the asymptotic approximation method as a semi-classical (quasi-classical) approximation, where results are most accurate in the nearly classical limit of large quantum numbers; These eigenvalues directly depend on the value of λ the most accurate results are obtained for large value of λ where λ is an integer or not (even or odd too).

6.0 CONCLUSION

The semi-classical (path-integral) approximation is the relatively simple Bohr-Sommerfeld condition for the energy spectrum in a quantitative manner in which the quantization procedure can be performed with these W.K.B.J. formulae (solutions). To get an estimate of the quality of the W.K.B.J approach to obtain the discrete energy values, it is interesting to compare the results with the exact results. There are no essential or remarkable differences between the exact eigenvalues and W.K.B.J. eigenvalues for modified Pöschl-Teller potential hole as n increases as well as λ The method (W.K.B.J) presented here is to serve as alternative that depends quantum mechanically on n and λ.

The accuracy of W.K.B.J approximation method is best assessed by comparing the W.K.B.J discrete energy values of this potential with those obtained either by solving the Schrödinger equation numerically, or whenever possible, using exact analytic expressions and since exact solution using this potential is possible we then used the exact analytic expressions to compare.

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