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New approximate radial wave functions for the modified Pöschl-Teller potential

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Satisfactory approximate radial wave functions are obtained for the modified Pöschl-Teller potential which simulates a quantum dot. The approximation is based on explicit summation of the leading constituent WKB series. Our approach reproduces the correct behaviour of the wave functions at the origin, at the turning points and far away from the turning points

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1. Introduction

In the present work we consider the modified Pöschl-Teller potential

$$V(r) = \frac{\hbar^2 k(k-1)}{2mR^2}\left(1 - \frac{1}{\cosh^2(r/R)}\right) = \frac{\hbar^2 k(k-1)}{2mR^2}\tanh^2(r/R) \tag{1}$$

which is assumed to be a confining quantum dot potential. This potential quickly tends to constant and leads to a finite number of energy levels. At the same time a confining potential is usually considered as hard-wall [1] or harmonic oscillator [2] potential. In these cases the number of energy levels is unphysically infinite.

The separated radial Schrödinger equation can be written in the form

$$-\hbar^2\frac{d^2\psi(r)}{dr^2} + 2m\left(V(r) + V_c(r) - E\right)\psi(r) = 0 \tag{2}$$

which is identical to the one-dimensional Schrödinger equation with an effective potential given by the sum of the origin potential $V(r)$ and the centrifugal potential

$$V_c(r) = \frac{\hbar^2 l(l+1)}{2mr^2}. \tag{3}$$

However this equation does not permit the exact solutions.

One of the earliest and simplest methods of obtaining approximate eigenvalues and eigenfunctions of the radial Schrödinger equation is the WKB method (see, e.g., [3, 4] and references therein). It is known [3, 5] that a suitable transformation of the initial equation improves results of an approximation technique. We examine the power-law substitutions

$$r = q^s, \quad s > 0, \quad \psi(r) = r^{(s-1)/2s}\Psi(q). \tag{4}$$

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The transformed equation is

$$-\hbar^2 \frac{d^2\Psi(q)}{dq^2} + Q(q)\Psi(q) = 0 \tag{5}$$

where

$$Q(q) = 2ms^2 \left(q^{2s-2} \left[\frac{\hbar^2 k(k-1)}{2mR^2} \tanh^2(q^s/R) - E \right] + \frac{\hbar^2}{2mq^2} \left[(l+1/2)^2 - \frac{1}{4s^2} \right] \right). \tag{6}$$

Of course, the exact solutions do not depend on some substitution. However, we are interesting in the approximate solutions. We apply the improved WKB method to equation (5), not to equation (2).

The WKB approach deals with the logarithmic derivative

$$Y(q) = \frac{d \ln \Psi(q)}{dq}, \quad \Psi(q) = c \exp\left(\int^q Y(q')dq' \right) \tag{7}$$

which satisfies the nonlinear Riccati equation

$$-\hbar^2 \left(\frac{dY(q)}{dq} + Y^2(q) \right) + Q(q) = 0 \tag{8}$$

where $Q(q)$ is an arbitrary function of q (naturally not only the special expression (6)). The WKB series

$$Y_{as}^{\pm}(q) = \hbar^{-1} \left(\pm Q^{1/2} + \sum_{n=1}^{\infty} \hbar^n Y_n^{\pm}(q) \right) \tag{9}$$

are the asymptotic expansions in powers of Plank's constant $\hbar$ of two independent particular solutions of the Riccati equation. The usual WKB approximations

$$Y_{WKB}^{\pm}(q) = \hbar^{-1} \left(\pm Q^{1/2} + \sum_{n=1}^{N} \hbar^n Y_n^{\pm}(q) \right) \tag{10}$$

contain a finite number of leading terms $Y_n^{\pm}(q)$ from the complete expansions $Y_{as}^{\pm}(q)$. These approximations are not valid at the turning points where $Q(q) = 0$ and at the origin $q = 0$. While in most cases of improvements of the WKB method (see, e.g., [4–7]) the main purpose is to achieve highest accuracy in eigenvalue calculation for the radial Schrödinger equation, our aim is to construct satisfactory approximate eigenfunctions with the correct behaviour at the origin, at the turning points and far away from the turning points.

2. New approximate logarithmic derivatives

The analysis of the well-known structure of leading $Y_n^{\pm}(q)$ and recursion relations [8, 9] allows us to reconstruct the asymptotic WKB series as the infinite sums

$$Y_{as}^{\pm}(q) = \pm\hbar^{-1} Q^{1/2} + \sum_{j=1}^{\infty} Z_{as,j}^{\pm}(q) \tag{11}$$

of new constituent (partial) asymptotic series $Z_{as,j}^{\pm}(q)$ [10, 11].

The complete series $Y^{\pm}_{as}(q)$ are approximated by a finite number of leading constituent series $Z^{\pm}_{as,j}(q)$ in contrast to the use of a finite number of leading terms $Y^{\pm}_n(q)$ in the conventional WKB approach. Using notation

$$a(q) = \frac{1}{\hbar^{2/3}} \frac{Q(q)}{|dQ(q)/dq|^{2/3}}, \tag{12}$$

$$b_1(q) = \frac{1}{\hbar^{2/3}} \frac{dQ(q)/dq}{|dQ(q)/dq|^{2/3}}, \quad b_2(q) = \frac{d^2Q(q)/dq^2}{dQ(q)/dq} \tag{13}$$

we are able to rewrite two first leading constituent series in the form

$$\pm\hbar^{-1}Q^{1/2} + Z^{\pm}_{as,1}(q) + Z^{\pm}_{as,2}(q) = b_1(q)y^{\pm}_{as,1}(a) + b_2(q)y^{\pm}_{as,2}(a). \tag{14}$$

Direct verification shows that the series $y^{\pm}_{as,1}(a)$ and $y^{\pm}_{as,2}(a)$ satisfy equations

$$\frac{dy^{\pm}_{as,1}}{da} + (y^{\pm}_{as,1})^2 = a, \tag{15}$$

$$\frac{dy^{\pm}_{as,2}}{da} + 2y^{\pm}_{as,1}y^{\pm}_{as,2} = \frac{1}{3}\left(2a\frac{dy^{\pm}_{as,1}}{da} - y^{\pm}_{as,1}\right). \tag{16}$$

Eq.(15) is the Riccati equation for the logarithmic derivatives of linear combinations of the well-studied Airy functions Ai(a) and Bi(a) [12]

$$y_1(a;t) = \frac{d}{da}\ln\left(\mathrm{Ai}(a) + t\mathrm{Bi}(a)\right). \tag{17}$$

Eq. (16) has the solution

$$y_2(a;t) = \frac{1}{30}\left[-8a^2(y_1(a;t))^2 - 4ay_1(a;t) + 8a^3 - 3\right] \tag{18}$$

As a result we get the new approximate logarithmic derivative

$$Y_{app}(q) = Y(q;t) = b_1(q)y_1(a;t) + b_2(q)y_2(a;t) \tag{19}$$

with a mixture parameter t. The function $Y(q;t)$ satisfies the following equation

$$-\hbar^2\left(\frac{dY(q;t)}{dq} + Y^2(q;t)\right) + Q(q) = -\hbar^2\left[\left(\frac{d^3Q(q)/dq^3}{dQ(q)/dq}\right)y_2(a;t)\right.$$
$$\left. + \left(\frac{d^2Q(q)/dq^2}{dQ(q)/dq}\right)^2 (y_2^2(a;t) - \frac{8}{3}y_2(a;t) + \frac{4}{3}ay_1(a;t)y_2(a;t) - \frac{1}{6})\right] \tag{20}$$

instead of equation (8).

The particular expressions

$$y_1^{\pm}(a) = y(a;\pm i) \tag{21}$$

and

$$y_1^{-}(a) = y(a;0), \quad y_1^{+}(a) = y(a;\infty) \tag{22}$$

correspond to the conventional WKB series .

It is not surprising that the asymptotics of our approximation coincide with the WKB asymptotics far away from the turning points. At the same time our approximation reproduces the known [9] satisfactory approximation near the turning points.

3. New approximate radial wave functions

Now we can construct the approximate radial wave functions for the bound states in the case of the modified Pöschl-Teller potential when $Q(q)$ is of the form (6).

First, we must reproduce the correct limiting behaviour at the origin. In this case we have following exact expressions ($r \to 0, q \to 0$)

$$\psi_{ex}(r) \to r^{l+1}, \quad \Psi_{ex}(q) \to q^{sl+(s+1)/2}, \quad Y_{ex}(q) \to \frac{sl+(s+1)/2}{q}. \tag{23}$$

At the same time we can derive relations

$$a(q) \to a_0 = \left(\frac{s^2}{4}(l+1/2)^2 - \frac{1}{16}\right)^{1/3}, \quad b_1(q) \to -\frac{2a_0}{q}, \quad b_2(q) \to -\frac{3}{q},$$

$$Y(q;t) \to -\frac{1}{q}\left(2a_0 y_1(a_0;t) + 3y_2(a_0;t)\right) \tag{24}$$

in the framework of our approach. We obtain the algebraic equation for determining the value of t. Its solution is

$$t_0 = \frac{-c(l,s)\mathrm{Ai}(a_0) + a_0(d\mathrm{Ai}(a_0)/da_0)}{c(l,s)\mathrm{Bi}(a_0) - a_0(d\mathrm{Bi}(a_0)/da_0)} \tag{25}$$

where

$$c(l,s) = 1 - \sqrt{1 + \frac{5}{4}\left(\frac{8a_0^3 - 3}{10} + s(l+1/2) + 1/2\right)}.$$

Two real turning points q_- and q_+ ($Q(q_\pm) = 0$) separate three regions.

In the first region where $0 < q < q_-$ we select the unique approximate particular logarithmic derivative $Y(q;t_0)$. In the second region where $q_- < q < q_+$ we must describe the oscillatory solution of the original Schrödinger equation (2). Therefore in this case we select two approximate particular logarithmic derivatives $Y(q;+i)$ and $Y(q;-i)$. In the third region where $q > q_+$ we must describe only the decreasing solution of the original Schrödinger equation (2). Therefore in this case we select the approximate particular logarithmic derivative $Y(q;0)$ or $Y(q;\infty)$ in accordance with sing of $dQ(q)/dq$. Note that in the case $l = 0, s = 1$ we put $q_- = 0$.

Since in our approach the turning points are ordinary nonsingular points, no question of connection formulas arises in contrast with the conventional WKB method. Matching particular solutions at the turning points we obtain the continuous approximate radial wave function

$$\psi_{app}(r) = N_{app} r^{(s-1)/2s} \Psi_{app}(q) \tag{26}$$

where $\Psi_{app}(q)$ is represented by the following formulas

$$\Psi_1(q) = \cos\phi_0 \exp\left(-\int_q^{q_-} Y(q';t_0)\,dq'\right) \tag{27}$$

if $0 < q < q_-$,

$$\Psi_2(q) = \exp\left(\int_{q_-}^{q} \frac{Y(q';+i) + Y(q';-i)}{2}\,dq'\right)$$
$$\times \cos\left(\int_{q_-}^{q} \epsilon \frac{Y(q';+i) - Y(q';-i)}{2i}\,dq' - \phi_0\right) \tag{28}$$

if $q_- < q < q_+$,

$$\Psi_3(q) = \frac{1}{2}(-1)^n \exp\left(\int_{q_-}^{q_+} \frac{Y(q';+i)+Y(q';-i)}{2}\, dq'\right)$$
$$\times \exp\left(\int_{q_+}^{q} \left[\frac{Y(q';\infty)+Y(q';0)}{2} - \epsilon\frac{Y(q';\infty)-Y(q';0)}{2}\right] dq'\right) \tag{29}$$

if $q > q_+$. Here $q = r^{1/s}$, $\phi_0 = \frac{\pi}{3} - \arctan t_0$, $\epsilon = \frac{dQ(q)/dq}{|dQ(q)/dq|}$ and N_{app} is a normalization constant.
We have the new quantization condition

$$\int_{q_-}^{q_+} \epsilon\frac{Y(q;+i)-Y(q;-i)}{2i}\, dq = \pi(n+\frac{1}{3}) + \phi_0, \quad n = 0,1,2... \tag{30}$$

which determines the spectral value of E implicitly.

Note that up to now a value of a substitution parameter s is not fixed. Numerical experiment for the modified Pöschl-Teller potential shows that the best choice for $l = 0$ is $s = 1$ and the satisfactory common choice for all $l > 0$ is $s = 2$. Thus the approximate eigenfunctions are determined completely and we can perform application.

4. Application of the proposed approximation

It is convenient to apply our approximation with introducing the dimensionless quantities

$$x = \frac{r}{R}, \quad e = \left(\frac{2mR^2}{\hbar^2}\right) E, \tag{31}$$

when the Schrödinger equation is rewritten in the form $\hat{H}\psi(x) - e\psi(x) = 0$ with the Hamiltonian

$$\hat{H} = -\frac{d^2}{dx^2} + V(x) + \frac{l(l+1)}{x^2}, \quad V(x) = k(k-1)\tanh^2(x). \tag{32}$$

Figures 1,2,3 demonstrate continuity of the proposed approximate radial wave functions and their derivatives in the case $k = 10$. Here solid lines reproduce normalized $\psi_{app}(x)$ and dashed lines reproduce $d\psi_{app}(x)/dx$.

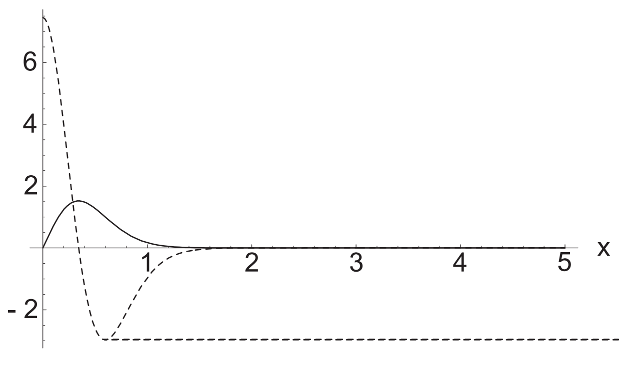

FIG. 1: Radial wave function and its derivative for $l = 0, n = 0$.

We calculate relative virial error

$$v = \frac{<\psi_{app}| -\frac{d^2}{dx^2} + \frac{l(l+1)}{x^2}|\psi_{app}>}{<\psi_{app}|\frac{1}{2}x\frac{dV(x)}{dx}|\psi_{app}>} - 1 \tag{33}$$

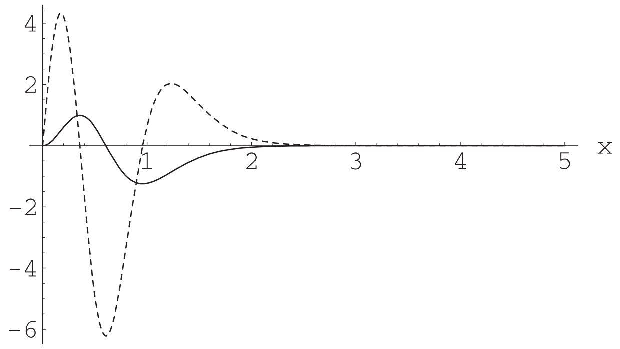

FIG. 2: Radial wave function and its derivative for $l = 1, n = 1$.

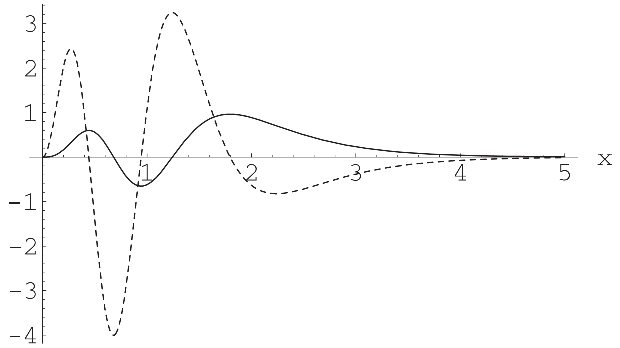

FIG. 3: Radial wave function and its derivative for $l = 2, n = 2$.

with the help of the normalized approximate wave functions ($<\psi_{app}|\psi_{app}>= 1$). v is equal to zero for the exact solutions.

We can also calculate the expectation values

$$e_{app} =<\psi_{app}|\hat{H}|\psi_{app}> \tag{34}$$

and $<\psi_{app}|\hat{H}^2|\psi_{app}>$. It should be stressed that $<\psi_{app}|\hat{H}|\psi_{app}>^2 \neq <\psi_{app}|\hat{H}^2|\psi_{app}>$ when the wave functions are not exact. Now we define the relative discrepancy

$$d = \frac{<\psi_{app}|\hat{H}^2|\psi_{app}>}{<\psi_{app}|\hat{H}|\psi_{app}>^2} - 1. \tag{35}$$

We estimate our approximation by means of the values of v and d. Our predictions are the values of energy e_{app}. The number of bound states depends on a value of a potential parameter k. If $k = 10$ then we have 15 bound states but if $k = 5$ we have only 3 states. Table 1 demonstrates validity of our approximation. In the particular case $l = 0$ we can compare our values of e_{app} and the exact energies e_{exact} from [13]. For $k = 10$ we have $e_{exact} = 26, 54, 74, 86$. In this case our approximation gives the high accuracy.

Table 1: Properties of the proposed approximation ($k = 10$).

l	n	v	d	e_{app}
0	0	$1.86 \cdot 10^{-2}$	$2.38 \cdot 10^{-4}$	26.0025
0	1	$8.23 \cdot 10^{-3}$	$5.14 \cdot 10^{-6}$	54.0004
0	2	$6.56 \cdot 10^{-3}$	$7.48 \cdot 10^{-7}$	74.0001
0	3	$6.79 \cdot 10^{-3}$	$3.32 \cdot 10^{-7}$	86.0000
1	0	$3.01 \cdot 10^{-2}$	$1.38 \cdot 10^{-2}$	41.6859
1	1	$1.44 \cdot 10^{-2}$	$1.02 \cdot 10^{-4}$	65.5729
1	2	$1.13 \cdot 10^{-2}$	$4.34 \cdot 10^{-5}$	81.4828
1	3	$1.08 \cdot 10^{-2}$	$1.31 \cdot 10^{-5}$	89.2997
2	0	$1.36 \cdot 10^{-2}$	$5.72 \cdot 10^{-3}$	55.8579
2	1	$8.30 \cdot 10^{-3}$	$2.16 \cdot 10^{-5}$	79.6009
2	2	$7.80 \cdot 10^{-3}$	$2.77 \cdot 10^{-6}$	87.2306
3	0	$7.41 \cdot 10^{-3}$	$2.75 \cdot 10^{-3}$	68.4940
3	1	$6.09 \cdot 10^{-3}$	$1.33 \cdot 10^{-5}$	83.9108
4	0	$4.17 \cdot 10^{-3}$	$1.37 \cdot 10^{-3}$	79.4497
5	0	$2.22 \cdot 10^{-3}$	$6.58 \cdot 10^{-4}$	88.4510

5. Conclusion

We see that the performed reconstruction of the WKB series and subsequent explicit summation of the leading constituent (partial) series yield the satisfactory (qualitative and quantitative) description of wave functions in the case of the radial Schrödinger equation with the modified Pöschl-Teller potential. The new way of using the old WKB series allows us to avoid all known difficulties of the conventional WKB approach.

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