Transition states and the critical parameters of central potentials

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Abstract
Transition states or quantum states of zero energy appear at the boundary between the discrete part of the spectrum of negative energies and the continuum part of positive energy states. As such, transition states can be regarded as a limiting case of a bound state with vanishing binding energy, emerging for a particular set of critical potential parameters. In this work, we study the properties of these critical parameters for short-range central potentials. To this end, we develop two exact methods and also utilize the first- and second-order WKB approximations. Using these methods, we have calculated the critical parameters for several widely used central potentials. The general analytic expressions for the asymptotic representations of the critical parameters were derived for cases where either the orbital quantum number $l$ or the number $n$ of bound states approaches infinity. The above mathematical models enable us to answer the following physical (quantum mechanical) questions. (i) What is the number of bound states for a given central potential and given orbital quantum number $l$? (ii) What is the maximum value of $l$ which can provide a bound state for the given central potential? (iii) What is the order of energy levels for the given form of the central potential? It is revealed that the ordering of energy levels depends on the potential singularity at the origin.

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(Some figures in this article are in colour only in the electronic version)

1. Introduction

It is generally agreed that estimating the number of bound states of the Schrödinger equation is a problem of great practical importance. A substantial effort was devoted to evaluating the upper and lower limits on the number of bound states for a given central potential. Bargmann [1] and Schwinger [2] seem to be the first who tackled this problem. Since then many authors...
have contributed to the study of this problem. Among them we would like to refer to the works [3–7] and to emphasize particularly the contribution of Calogero and Brau [8–12].

The purpose of the current contribution is to present a systematic approach to the investigation of quantum states with zero energy. These transition states appear between the discrete part of the spectrum of negative energies and the continuum part of positive energies. We study transition states by solving the proper Schrödinger equation for short-range central potentials possessing specific sets of critical parameters. To this end, we develop two exact methods for solving the zero-energy Schrödinger equation, and for obtaining the values of the associated critical parameters. We apply these methods to find the critical parameters of an important class of central potentials including among others the Gaussian and the Yukawa interactions. A few examples of potentials admitting the analytic solutions for the transition states are exhibited and the associated critical parameters are presented in analytic form. We provide numerical results in the form of tables of the critical parameters. These results enable one to obtain the exact number of bound states for these potentials without any additional computations.

Analyzing our results we have observed the following universal properties of the solutions of the Schrödinger equation with central potentials. (a) For a given orbital angular momentum quantum number \(l\), the \(n\)th critical value of the universal parameter \(\beta_{n,l}\) of any potential behaves as \(n^2\) for large \(n\). (b) For a given number \(n\) of bound states, the critical parameter \(\beta_{n,l}\) grows as \(l^2\) with increasing \(l\). Both results can be explained with the help of the WKB approximation. (c) The ordering of the energy levels with various \([n, l]\) depends on the potential singularity at the origin.

The paper is organized as follows. In section 2, we briefly discuss the Schrödinger equation and the properties of short-range potentials. The asymptotic behavior of the solution at the origin and at infinity is discussed in sections 3 and 4, respectively. In section 5, we introduce a phase-kind equation for the transition states, and in section 6, we describe the WKB approximations for the calculation of the critical parameters. The analytic asymptotic expressions for the critical parameters are presented in section 7. Numerical results and conclusions then follow in sections 8 and 9.

2. Short-range potentials

Let us start this section with a quotation from section 18 in the Landau and Lifshitz textbook on quantum mechanics [13]: 'If the field diminishes as \(-1/r^s\) at infinity, with \(s > 2\), then there are no levels of arbitrarily small negative energy. The discrete spectrum terminates at a level with a non-zero absolute value, so that the total number of levels is finite'.

The results of this paper enable us to doubt in the universal character of the statement expounded in the first sentence of the above quotation. The conclusion made in the second sentence proves to be true.

Therefore, we shall consider the central potentials \(V(r)\) satisfying the corresponding boundary condition at infinity:

\[
\lim_{r \to \infty} r^2 V(r) = 0. \tag{1}
\]

Near the origin, the boundary condition for an attractive potential can be written in a similar form

\[
\lim_{r \to 0} r^2 V(r) = 0, \tag{2}
\]

to avoid fall of a particle to the center [13] (sections 18 and 35).
We shall consider the class of potentials which can be presented in the form
\[ V(r, r_0) = -\frac{g}{r^s} f\left(\frac{r}{r_0}\right) \quad (g > 0, r_0 > 0), \]  
(3)
where \( g \) is the coupling constant which determines the strength of the interaction. Note that according to condition (2), the power \( s \) must satisfy the inequality
\[ q = s + p < 2, \]  
(4)
where \( p \) corresponds to the leading term in series expansion of function \( f(r) \) near the origin
\[ f(r) \sim \frac{\tilde{g}}{r^p}. \]  
(5)
It should be realized that definition (3) describes a wide class of potentials such as, e.g., square well, exponential, Hulthen, Gaussian, Yukawa, Woods–Saxon and many others.

The radial part of the Schrödinger equation for a single particle moving in a central potential field takes the form [13](section 32)
\[ \frac{d^2 \chi}{dr^2} + \left\{ \frac{2m}{\hbar^2} E - V(r) - \frac{l(l+1)}{r^2} \right\} \chi = 0, \]  
(6)
where \( m \) is the reduced mass and \( \chi \equiv \chi_l(r) \) is the reduced radial part of the wavefunction for a stationary state with angular momentum \( l \) and energy \( E \).

Changing the potential parameters, the appearance of a new bound state is accompanied with a new solution of equation (6) for \( E = 0 \). As we limit our discussion to potentials of the form (3), we rewrite equation (6) for zero energy in the form
\[ \frac{d^2 \tilde{\chi}}{dx^2} = \left[ -\frac{2m}{\hbar^2} \frac{g}{r^s} f\left(\frac{r}{r_0}\right) + \frac{l(l+1)}{x^2} \right] \tilde{\chi}(x). \]  
(7)

The scale transformation \( x = r/r_0 \) leads to the equation
\[ \frac{d^2 \tilde{x}}{dx^2} = \left[ -\frac{2m}{\hbar^2} \frac{g}{r_0^{2-s}} f(x) + \frac{l(l+1)}{x^2} \right] \tilde{x}(x). \]  
(8)

It is seen that the potentials \( V(r, r_0) \) and \( r_0^{2-s}V(r, 1) \) have equivalent solutions of equation (6). Thus, we are interested in solving the equation
\[ \chi''(r) = U(r)\chi(r), \]  
(9)
where
\[ U(r) = -\beta v(r) + \frac{l(l+1)}{r^2}, \]  
(10)
\[ v(r) = f(r)r^{-s}. \]  
(11)
Now our choice of the form (3) for central potentials becomes clear. The solutions of equation (9) for a given angular momentum quantum number \( l \) depend effectively, (see, e.g., [14]) only on one parameter
\[ \beta = \frac{2mg}{\hbar^2 r_0^{2-s}}. \]  
(12)
Equation (9) is a differential equation of second order. In order to solve it both analytically and numerically, one needs to know the behavior of its solution near the origin and at infinity.
3. The solution near the origin

At first, let us consider the solution of equation (9) near the origin. Expanding the potential into a power series and keeping only the leading term, we obtain

\[ \chi''(r) = \left[ -\frac{\lambda}{r^q} + \frac{l(l+1)}{r^2} \right] \chi(r), \]  

(13)

where

\[ \lambda = \beta \tilde{g}, \]  

(14)

and \( q \) is defined by equation (4). The particular solution of equation (13), satisfying the boundary condition

\[ \chi(0) = 0, \]  

(15)

has the form

\[ \chi(r) = A \sqrt{r} J_{2l+1} \left( \frac{2\sqrt{\lambda}}{2-q} r^{1-q/2} \right), \]  

(16)

where \( J_n(z) \) is the Bessel function of the first kind and \( A \) is an arbitrary constant. Keeping the first two terms in the series expansion of the function (16), one obtains

\[ \chi(r) \approx A r^{l+1} \left[ \frac{2\sqrt{\lambda}}{2-q} r^{1-q/2} \right]. \]  

(17)

In general, for integer and half-integer \( q \), the solution of equation (9) satisfying the boundary condition (15) can be presented by the following infinite series:

\[ \chi(r) = A r^{l+1} \left[ 1 + \sum_{i=1}^{\infty} r^i (b_i + r^{1-q} c_i) \right]. \]  

(18)

For integer \( q \), all of the \( b \)-coefficients should be zero. It follows from equation (17) that

\[ c_1 = -\frac{\lambda}{(2-q)(2l+3-q)}. \]  

(19)

Substituting representation (18) into equation (9), and then equating the expansion coefficients of the same powers of \( r \) for the left-hand (lhs) and right-hand sides (rhs) of equation (9), one can calculate any finite number of the subsequent coefficients \( c_i \) and \( b_i \) with \( i \geq 1 \).

4. The asymptotic behavior of transition states

For an eigenfunction \( \Psi \) belonging to the discrete part of the spectrum, the integral \( \int |\Psi|^2 dV \), taken over all space, is finite. This certainly means that \( |\Psi|^2 \) decreases quite rapidly, becoming zero at infinity. ‘The system executes a finite motion, and is said to be in a bound state’ [13] (section 10). For wavefunctions belonging to the continuous part of the spectrum, the integral \( \int |\Psi|^2 dV \) diverges due to the fact that \( |\Psi|^2 \) does not become zero at infinity (or becomes zero insufficiently rapidly).

On the other hand [13] (section 18), the spectrum of negative eigenvalues of the energy is discrete, i.e. all states with \( E < 0 \) in the field which vanishes at infinity are bound states. The positive eigenvalues \( E > 0 \), on the other hand, form a continuous spectrum.

In other words, for the bound states, the eigenvalues of the energy \( E < 0 \) and the eigenfunctions must satisfy the boundary condition

\[ \lim_{r \to \infty} |\Psi|^2 = 0. \]  

(20)
In contrary, for a free state that belongs to the continuous spectrum, the energy eigenvalues $E > 0$ and $|\Psi|^2$ does not become zero at infinity (or becomes zero insufficiently rapidly).

For the transition states with $E = 0$, the asymptotic behavior ($r \to \infty$) of the eigenfunctions remains unclear.

The important step is to realize that the boundary condition (20) must be valid for the transition states ($E = 0$) as well. Thus, for these states, $|\Psi|^2$ achieves zero at infinity. However, we note that it may tend to zero too slowly to ensure the convergence of the integral $\int |\Psi|^2dV$.

In the following we shall rely on the boundary condition (20) for the transition states.

For $l > 0$, the asymptotic boundary condition (1) enables us to neglect the potential $V(r) = -\beta v(r)$ in equations (9)–(11) at large enough $r$. The general solution of the resulting equation has a form

$$\chi_l(r) = C_1r^{l+1} + C_2r^{-l},$$

where $C_1$ and $C_2$ are arbitrary constants. As $\Psi \sim R(r) = \chi_l(r)/r$, one should put $C_1 = 0$ in order to satisfy the asymptotic condition (20). Thus, we obtain

$$\chi_l(r) \xrightarrow{r \to \infty} C_2r^{-l}. \quad (22)$$

Expressing the latter equation in the form $r^l\chi_l(r) \xrightarrow{r \to \infty} \text{const}$, we obtain the following condition for the first derivative:

$$\lim_{r \to \infty} \frac{d}{dr}[r^l\chi_l(r)] = \lim_{r \to \infty} [lr^{l-1}\chi_l(r) + rl^{l-1}\chi'_l(r)] = 0. \quad (23)$$

It is clear that the asymptotic behavior of the solution $\chi_l(r)$ of equation (9) depends on the parameter $\beta$ of the effective potential (10). Thus, according to equation (23), the solution $\chi_l$ of equation (9) fulfills the asymptotic condition

$$F_l(\beta_n) = \lim_{r \to \infty} \left[ l r^{-l} \chi_l(r) + \chi'_l(r) \right] = 0 \quad (24)$$

for the critical parameters $\beta_n$. Here $n$ is a number of zeros of the function $F_l(\beta)$ for the given potential (10). Hence, by definition, if for a given $l$ the potential $V(r)$ is characterized by the parameters meeting $\beta_{n+1} \geq \beta > \beta_n$, then the proper number of bound states equals $n$.

The asymptotic condition (24) was derived assuming that the orbital quantum number $l > 0$. However, it is easy to show that equation (24) preserves its validity also for $l = 0$. A typical graph of the function $F_l(\beta)$ is presented in figure 1.

The straightforward solution of the second-order differential equation (9) with the boundary conditions (17) and (24) presents our first method for calculating the critical parameters $\beta_n$ of a given attractive potential (3) satisfying the boundary conditions (1) and (2). This method is especially effective and accurate for small values of $l$. For a few potentials, such as the exponential, the Hulthen and the Woods–Saxon, one can derive analytical expressions for the critical parameters using this method (see the appendix). However, this is possible only for $S$-states ($l = 0$), when equation (9) with the potentials mentioned above has a general analytical solution. We are familiar with only one form of central potential which admits an analytical solution of equation (9) for $l \geq 0$. It is a cut-off potential (described in the appendix) for which the finite square well potential presents its particular case.

Let us add one important comment. We refer to equation (24) as the asymptotic behavior condition. However, solution (21), and therefore—condition (24), correspond to the assumption that the potential $V(r)$ is negligible in comparison with the centrifugal term $l(l + 1)/r^2$. Therefore, condition (24) is applicable at a distance $r$ when the condition

$$|V(r)| \ll \frac{l(l + 1)}{r^2} \quad (25)$$

is satisfied.
Figure 1. Function $F_0(\beta) = \lim_{r \to \infty} \chi_0'(r)$ for the Yukawa potential ($l = 0$). Zeros of $F_0(\beta)$ present critical parameters $\beta_n$.

5. Equation of the phase kind

It was mentioned in the preceding section that the straightforward method for calculating the critical parameters of central potentials loses its accuracy with increasing angular momentum quantum number $l$. In this section, we propose another method for calculating these parameters. This method is based on the logarithmic derivative $y(r) = \chi'(r)/\chi(r)$ of the reduced radial wavefunction introduced earlier. The final equations are close to but differ from the so-called phase equations presented in [10, 12].

Let us start with the trivial identity
\[
\left( \frac{\chi'}{\chi} \right)' = \frac{\chi''}{\chi} - \left( \frac{\chi'}{\chi} \right)^2, \tag{26}
\]
and transform the radial Schrödinger equation (9) into a Riccati-type equation for the corresponding logarithmic derivative $y(r) \equiv y_l(r)$:
\[
y'(r) + \gamma^2(r) = U(r). \tag{27}
\]
The asymptotic behavior of the logarithmic derivative for $l > 0$
\[
y_l(r) \overset{r \to \infty}{\sim} \frac{l}{r} \quad (l > 0) \tag{28}
\]
follows from the asymptotic representation (22).

To deduce the asymptotic behavior of the logarithmic derivative for the transition $S$-states ($l = 0$), let us start with the fact that for this case the rhs of equation (27) equals $V(r)$. Let us then consider central potentials with the asymptotic behavior
\[
V(r) \overset{r \to \infty}{\sim} -\frac{\beta}{r^\mu} \quad (\beta > 0), \tag{29}
\]
where $\mu > 2$ according to the boundary condition (1). The general solution of the proper Schrödinger equation (9) has a form
\[
\chi(r) = \sqrt{7} [C_2 J_\nu(2\sqrt{\beta r}) + C_3 J_{-\nu}(2\sqrt{\beta r})], \tag{30}
\]
with
\[ v \equiv \frac{1}{2 - \mu} < 0 \quad (\mu > 2). \tag{31} \]

It is seen that for \( \mu > 2 \), the argument of the Bessel function goes to zero as \( r \to \infty \). Thus, using series expansion for the Bessel functions, it is easy to show that one should put \( C_2 = 0 \) in order to satisfy the boundary condition \( (20) \). Taking then the logarithmic derivative for the resulting \( \chi (r) \), and once more using a series expansion for the Bessel functions, one obtains
\[ y_0(r) \approx \frac{\beta}{r^{1-\mu}}. \tag{32} \]

It is clear that the asymptotic solution \( (32) \) of the Riccati equation \( (27) \) for \( l = 0 \) satisfies the following inequality:
\[ y_0(r) \ll \beta \text{e}^{-r}. \tag{33} \]

The asymptotic solution of the Schrödinger equation \( (9) \) with the exponential potential is presented in the appendix (see equation \( (A.20) \)) for \( l = 0 \). The corresponding logarithmic derivative
\[ y_0^{\text{exp}}(r) \approx \beta \text{e}^{-r} \tag{34} \]
satisfies inequality \( (33) \). It is easy to show that the asymptotic representation \( (r \to \infty) \) of the Hulthen and the Woods–Saxon potentials reduces to the exponential forms \( -\beta \text{e}^{-r} \) and \( -\beta x_0^{-1} \text{e}^{-r} \), respectively. Hence, the asymptotic solution of the corresponding equation \( (27) \) can be presented by the rhs of equation \( (34) \) for the Hulthen potential, and by \( \beta x_0^{-1} \text{e}^{-r} \) for the Woods–Saxon potential. The latter logarithmic derivatives certainly obey inequality \( (33) \) as well.

It is reasonable to suggest that inequality \( (33) \) is valid for all the short-range potentials (may be excluding only the cut-off potentials). In this case, one can neglect the square of the logarithmic derivative in the lhs of equation \( (27) \). The solution of the latter equation with \( l = 0 \) can be obtained then in the explicit form
\[ y_0(r) \approx \beta \int_r^\infty v(r) \, dr. \tag{35} \]

For potentials with the asymptotic behavior \( (29) \), formula \( (35) \) gives the asymptotic representation \( (32) \). For the exponential potential, the rhs of equation \( (35) \) leads to \( (34) \).

For the Yukawa and Gaussian potentials, equation \( (35) \) yields
\[ y_0^{\text{Yuk}}(r) \approx \beta \text{e}^{-r}, \quad y_0^{\text{Gau}}(r) \approx \frac{\beta}{2} \text{e}^{-r}. \tag{36} \]

For deriving the latter expressions, we used the leading terms of the asymptotic expansions of the incomplete gamma function \( \Gamma(0, r) \) and the complementary error function \( \text{erfc}(r) \) obtained as the results of integration in equation \( (35) \).

It is easy to check that the asymptotic logarithmic derivatives \( (36) \) satisfy inequality \( (33) \). The substitution
\[ y_0(r) = K(r) \cot \eta(r) \tag{37} \]
enables us to transform equation \( (27) \) into the following equation for the phase function \( \eta(r) \):
\[ \eta'(r) = \frac{K'(r)}{2K(r)} \sin 2\eta(r) + K(r) \cos^2 \eta(r) = \frac{U(r)}{K(r)} \sin^2 \eta(r). \tag{38} \]
The stabilizing function $K_r$ can be chosen in a sufficiently arbitrary manner. The simplest choice is $K_r = 1$. In this case, the boundary conditions (28) and (35) define the following asymptotic condition for $\eta(r)$:

$$\eta(\infty) = -\pi/2 + n\pi \quad (n = 1, 2, \ldots).$$  \hfill (39)

Any function $K_r$ that preserves the limit, $\lim_{r \to \infty} [y(r)/K(r)] = 0$, provides the asymptotic behavior (39). It was established (at least numerically) that the more precise results are provided by stabilizing functions of the form

$$K_r = \sqrt{U_l(r)},$$  \hfill (40)

where $U_l(r)$ governs the behavior of $U(r)$ both near the origin and at infinity, that is,

$$U_l(r) =
\begin{cases} 
\beta v(r), & l = 0 \\
\beta u(l(r) + 1)r^{-2}, & l > 0.
\end{cases}$$  \hfill (41)

Use of the stabilizing functions (40) and (41) enables us to replace equation (38) with two simpler equations:

$$\eta'(r) = \frac{U'_l(r)}{4U_l(r)} \sin 2\eta(r) + \sqrt{U_0(r)} \quad (l = 0),$$  \hfill (42)

$$\eta'(r) = \frac{1}{r} \left[ \sqrt{l(l+1)} \cos 2\eta(r) - \frac{1}{2} \sin 2\eta(r) \right] + \frac{rU_0(r)}{\sqrt{l(l+1)}} \sin^2 \eta(r) \quad (l > 0).$$  \hfill (43)

Substituting expressions (40) and (41) for $l > 0$ into definition (37) with the asymptotic form (28), one obtains $\cot \eta(\infty) = -\sqrt{l/(l+1)}$. Thus, the critical parameters $\beta_n$ must provide the following asymptotic behavior for the function $\eta(r)$:

$$F_l(\beta_n) \equiv \eta(\infty)|_{\beta=\beta_n} = \delta_l - \frac{\pi}{2} + n\pi \quad (n = 1, 2, \ldots),$$  \hfill (44)

with

$$\delta_l = \arctan \left[ \sqrt{l/(l+1)} \right].$$  \hfill (45)

Equation (44) was derived for $l > 0$. It describes the asymptotic behavior of the solutions of equation (43). However, it is clear that the stabilizing function $K_0(r) = \sqrt{U_0(r)}$ preserves the correctness of the asymptotic formula (39) for the logarithmic derivatives $y_0(r)$ with the asymptotic behavior defined by equation (35). Therefore, condition (44), (45) with $l = 0$ can also be used for the asymptotic approximation of solutions of equation (42).

It is seen from equation (42) that the stabilizing function $K_0(r) = \sqrt{U_0(r)}$ can be applicable only in the case of its nodeless character; otherwise the simplest choice is $K_0(r) = 1$.

The technique described above in this section is sufficient for the presentation of the second method for calculating the critical parameters of central potentials of the from (3). However, we would like to make some additional remarks that can be useful.

Equations (42) and (43), along with the boundary condition (44), (45), provide a stable and accurate solution to the problem of critical potentials for both small and large values of $l$.

A typical graph of function $t = F_l(\beta)$ has a staircase form. It is presented in figure 2. The abscissas of the points of the staircase function intersections with lines $t = \delta_l - \pi/2 + n\pi$ give the desired critical parameters $\beta = \beta_n$.

As an additional useful information, it can be shown that

$$F_l(0) = \delta_l.$$  \hfill (46)
Figure 2. Function $\tilde{F}_7(\beta) = \lim_{r \to \infty} \eta(r)$ for the Gaussian potential ($l = 7$). The abscissas of the points of intersection of $t = \tilde{F}_7(\beta)$ with lines $t = \delta_l - \pi/2 + \pi n$ give the desired critical parameters $\beta = \beta_n$.

This is because of the following. Setting $\beta = 0$, the second term disappears from the rhs of equation (42). The analytic solution to the resultant equation has a form

$$\eta(r) = \arctan(C \sqrt{U_0(r)}).$$

(47)

Condition (1) thus provides $\eta(\infty) = 0$ for $\beta = 0$ and $l = 0$ according to equation (47).

Putting $\beta = 0$ in equation (43), the latter loses the term with $U_0(r)$. The resultant equation has an analytic solution of the form

$$\eta(r) = \arctan \left( \frac{2l + 1}{2} \tanh \left( \frac{(2l+1)}{2} \ln r + C \right) - 1 \right).$$

(48)

For arbitrary finite real $C$, tanh presented in equation (48) approaches 1 as $r \to \infty$. The resultant expression thus reduces to $\delta_l$.

6. The first- and second-order WKB approximations

In this section, we apply the first-order and the second-order WKB approaches to calculating the critical parameters of central potentials. Unlike the exact methods presented earlier, these methods are certainly approximate but they are also much simpler.

Langer correction was not applied, because it was pointed out by several authors (see, e.g., [19]) that Langer’s replacement of $l(l+1)$ by $(l+1/2)^2$ is not valid for the second- and higher-order WKB approximations.

Specific modification of the first-order WKB approach presented below cannot provide results of high precision. However, its accuracy grows rapidly with increasing the number $n$ of bound states. It is important to note that this method can be formally applied to transition states with any orbital quantum number $l \geq 0$.

The accuracy of the second-order WKB method grows with increasing $l$. For example, the relative error for $l > 10$ can be less than $10^{-5}$. This enables one to test the results obtained
by the phase-kind method (section 5) for large $l$. On the other hand, the second-order WKB calculations can be formally performed for small values of $l$ too. The corresponding relative error was less than 50% even for $l = 1$. Thus, one can conclude that the WKB approximation can be used if very high accuracy is not needed. The disadvantage of this method is its inapplicability for the transition $S$-states ($l = 0$).

For $E = 0$, the presence of the centrifugal term in the effective potential $U(r)$ ensures the existence of two turning points for attractive potentials of the form (3). In the second-order approximation [16], the WKB quantization condition [17–19], as applied to our consideration, can be written as

$$S_0 + S_2 = \left( n - \frac{1}{2} \right) \pi \quad (n = 1, 2, \ldots),$$

where $n$ is the number of bound states as in the previous sections. The term

$$S_0 = \int_{r_1}^{r_2} \sqrt{-U(r)} \, dr \quad (50)$$

together with the term $S_1 = -\pi/2$ corresponds to the first-order WKB approximation (for two turning points). The turning points $r_1$ and $r_2$ are the roots of the equation

$$\frac{1}{l(l+1)} \frac{r_i}{r_i^2} = \beta v(r_i) \quad (i = 1, 2),$$

where the function $v(r)$ is defined by equations (3) and (11). The second-order correction takes the form [16, 18]

$$S_2 = \lim_{\mu \to +0} \left( \frac{1}{48} \int_{r_i}^{r_2 - \mu} \frac{U''(r)}{(-U(r))^{1/2}} \, dr - \frac{1}{12\sqrt{\mu}} (b_1|a_1|^{-3/2} + b_2|a_2|^{-3/2}) \right),$$

where $a_1, b_1, a_2$ and $b_2$ are the expansion coefficients of the effective potential $U(r)$ in the neighborhood of the turning points. That is,

$$U(r_i + \delta r) = a_0 \delta r + b_0 (\delta r)^2 + \cdots,$$

where from equation (51) it can be seen that

$$a_i = -\beta \left[ \frac{2}{r_i} v(r_i) + v'(r_i) \right],$$

$$b_i = \frac{1}{2} \beta \left[ \frac{6}{r_i^2} v(r_i) - v''(r_i) \right].$$

Note that in [16], the power affecting the potential $-U(r)$ in equation (52) was presented to be 2/3 by mistake. The correct power 3/2 can be found in [18].

One should emphasize that the small magnitude of the second-order correction (52) results from the difference of two large terms. Therefore, both these terms must be calculated with high accuracy. Nevertheless, we would like to stress that this correction increases the accuracy of the WKB approximation by two to three orders of magnitude.

A modification of the first-order WKB method, where the centrifugal potential is excluded from the quasiclassical momentum [28], can be applied for calculating the critical parameters under consideration. According to this approach, the quantization condition for the transition states ($E = 0$) reduces to

$$\int_0^\infty \sqrt{\beta v(r)} \, dr = \pi (n + \gamma_{l,q}),$$

where

$$\gamma_{l,q} = \begin{cases} 
\frac{2l - 1}{4}, & q \leq 0 \\
\frac{2l - 1 + q}{2(2 - q)}, & 0 < q < 2.
\end{cases}$$

(56)
In accordance with its definition (4), the parameter $q$ is ruled by the behavior of the central potential near the origin. The cut-off potential (A.1) presents an exclusion. The exact analytic solution for this case is presented in the appendix.

7. The critical parameter asymptotics

It was shown in the previous sections that in general the critical parameters for central potentials can be calculated numerically. For a few special cases, presented in the appendix, one can deduce the analytical results.

In this section, it will be shown that it is possible to derive the analytical expressions for the asymptotic form of the critical parameters $\beta_{\nu} \equiv \beta_{\nu,l}$. In doing so, asymptotic implies a situation where either the number of bound states $n$ approaches infinity for a given finite $l$, or the orbital angular momentum quantum number $l$ goes to infinity for a given finite $n$.

It is well known that the accuracy of the WKB method increases for higher excitations (large $n$). It follows from section 49 of [13] that the first-order WKB approximation is almost perfectly suitable for considering the limit case of $l \to \infty$, as well. Thus, the first-order WKB approach is applied to solve the problem of $\beta_{\nu,l}$-asymptotics.

First, let us consider the case of finite $n$ where $l \to \infty$.

Numerical calculations demonstrate that the distance between turning points $|r_1 - r_2|$ reaches zero as $l$ approaches infinity. This result can be explained and supported by the following arguments. According to equations (49) and (50), the standard Bohr–Sommerfeld quantization condition for the transition states reads

$$\int_{r_1}^{r_2} \sqrt{-U(r)} \, dr = \left( n - \frac{1}{2} \right) \pi. \quad (57)$$

This means that the effective potential $U(r)$ must be negative in the range $[r_1, r_2]$. Hence, according to equation (10), the critical parameter $\beta$ must tend to infinity as $l^2$ or faster for $l \to \infty$. The latter in turn implies that the integrand in the lhs of equation (57) approaches infinity as $l \to \infty$, whereas the rhs of equation (57) remains finite. The above contradiction can be eliminated only by setting $r_1 = r_2$ for the limits of integration, which proves the statement.

It is clear that the point $R_m$ of minimum of the effective potential $U(r)$ is localized in the region $[r_1, r_2]$, that is,

$$r_1 \leq R_m \leq r_2. \quad (58)$$

Therefore, when $l$ approaches infinity, $R_m$ tends to the point where the turning points $r_1$ and $r_2$ merge. Hence, in order to calculate $r_m = \lim_{l \to \infty} R_m$, it is enough to solve the following set of equations:

$$\begin{cases} U(r_m) = 0 \\ U'(r_m) = 0. \end{cases} \quad (59)$$

Substituting the explicit form (10) into (59) and eliminating $\beta$ and $l$, one obtains the following simple equation for $r_m$:

$$2v(r_m) + r_m v'(r_m) = 0. \quad (60)$$

Now, any of the two equations (59) gives the required asymptotic expression

$$\beta_{\nu,l} \simeq \frac{d_l}{2} (l + 1). \quad (61)$$

with

$$d_l = \frac{2}{r_m^2 v(r_m)}. \quad (62)$$
presented in Table 1 along with the values of $\frac{d\beta_{n,l}}{d\gamma_{l,q}}$. The numerical results for $\Delta_{n,l} = \beta_{n,l+1} - 2\beta_{n,l} + \beta_{n,l-1}$ and $\Delta_{n,l} = 2\beta_{n,l-1} - 2\beta_{n,l} + \beta_{n,l+1}$ are presented for comparison.

| Potential        | Exponential | Hulthen | Yukawa | Gaussian | WS $(\lambda_0 = 1)$ | WS $(\lambda_0 = 0.001)$ |
|------------------|-------------|---------|--------|----------|----------------------|--------------------------|
| $v(r)$           | $e^{-r}$    | $\left((e^r - 1)^{-1} e^{-r}/r\right)$ | $e^{-r^2}$ | $(1 + x_0 e^r)^{-1} (1 + x_0 e^r)^{-1}$ |                      |                          |
| $r_m$            | 2           | 1.59362 | 1      | 1        | 2.21772              | 6.17241                  |
| $d_0$            | $\frac{2}{3} / 3.69453 / 5.3865 / 7.5469 / (x_0 - 1)^2$ | $2e / 5.43656 / 5.43656 / 4.14202 / 0.077658$ | $4.14202$ | $0.077658$          |                      |                          |
| $\Delta_{1,19}$  | 5.69449     | 3.08828 | 2.64386 | 5.43639  | 4.14471              | 0.077846                  |
| $\Delta_{3,19}$  | 3.69674     | 3.08845 | 5.43698 | 5.4385   | 4.14471              | 0.077846                  |
| $\Delta_{5,19}$  | 4.88254     | 1.98432 | 3.11141 | 12.5151  | 6.29585              | 0.286015                  |
| $\Delta_{9,19}$  | 4.9300      | 1.9982  | 3.138   | 12.561   | 6.347                | 0.2868                    |

The second derivatives $d_l = d^2\beta_{n,l}/dl^2$ of the asymptotic critical parameters (61) are presented in Table 1 along with the values of $\Delta_{n,l} = \beta_{n,l+1} - 2\beta_{n,l} + \beta_{n,l-1}$ which approximate the general second derivative $d^2\beta_{n,l}/dl^2$ numerically. It is seen from this table that the values of $d_l$ are very close to the values of $\Delta_{1,19}$ for the lowest (nodeless) energy states ($n = 1$) and $l = 19$. It is worth noting that even though the Yukawa and Gaussian potentials are very different, their asymptotic behaviors are coincident ($d_l = 2e$).

Note that a set of equations (59) for calculating $r_m$ cannot be applied to the cut-off potential (A.1). The correct result (A.24) can be obtained by setting $r_m = 1$, that is, by equating the merging point $r_m$ and the matching point $r = 1$.

Now let us consider the case of $n \to \infty$ ($l$ is finite). To this end, one can successfully employ the modified WKB method [28] presented in the previous section. According to the authors of [28], their method is "exact in the asymptotic limit $n_r \to \infty \neq \Delta_{n_r} \to \infty", where $n_r = n - 1$. Our numerical results confirm this assertion. Thus, using directly the quantization condition (55), one obtains

$$\beta_{n,l} \sim \frac{d_n}{n} (n + \gamma_{l,q})^2, \quad \text{(63)}$$

where

$$d_n = 2 \left( \frac{\pi}{\int_0^\infty \sqrt{v(r)} dr} \right)^2, \quad \text{(64)}$$

and the parameter $\gamma_{l,q}$ is defined in equation (56).

For the FSW-like potential, equation (64) gives $d_n = 2\pi^2 \left( \frac{\gamma_{l,q}}{\beta_{n,l}} \right)^2$, which certainly coincides with the analytic solution presented in the first section of the appendix. In general, it is easy to check that the asymptotic expressions for the analytic solutions presented in the appendix coincide with the results of this section.

It is clear that formula (64) is correct only for a function $v(r)$ of constant (positive) sign that yields only two turning points. All the potentials considered in this work possess this property.
Table 2. Critical parameters $\beta = 2m\gamma^2\hbar^2$ of the exponential potential $V(r) = -g \exp(-r/r_0)$.

| $n$ | 0 | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 |
|-----|---|---|---|---|---|---|---|---|---|
| 1   | 1.4457965 | 7.0490613 | 16.312928 | 29.258323 | 45.892427 | 66.218077 | 90.236557 | 117.94852 | 149.35431 |
| 2   | 7.6178156 | 16.921126 | 29.879667 | 46.518231 | 68.345880 | 92.323660 | 120.00486 | 151.38676 | 185.24507 |
| 3   | 18.7215258 | 48.076670 | 68.345880 | 92.323660 | 120.00486 | 151.38676 | 185.24507 | 225.24507 | 259.90357 |
| 4   | 34.760071 | 50.947660 | 71.002111 | 94.837734 | 122.41832 | 153.72542 | 188.74853 | 227.48127 | 269.91954 |
| 5   | 55.730706 | 75.226301 | 98.713352 | 126.05709 | 157.19351 | 192.08825 | 230.72116 | 273.07970 | 319.15566 |
| 6   | 81.640838 | 104.38402 | 131.24653 | 162.04738 | 196.69590 | 235.14112 | 277.35218 | 323.30940 | 372.99967 |
| 7   | 112.48338 | 138.43438 | 168.62580 | 202.83958 | 240.96044 | 282.92106 | 328.67953 | 378.20847 | 431.48931 |
| 8   | 148.26072 | 177.38629 | 210.86809 | 248.45649 | 290.01388 | 335.45733 | 384.73391 | 437.80834 | 494.65627 |
| 9   | 188.97285 | 221.24597 | 257.98574 | 298.91536 | 343.87710 | 392.77335 | 445.54045 | 502.13521 | 588.50907 |
| 10  | 234.61978 | 270.01793 | 309.98801 | 354.22957 | 402.56672 | 454.88817 | 511.11996 | 588.50907 | 683.54571 |
| 11  | 285.20151 | 323.70558 | 366.88206 | 414.40969 | 466.09616 | 521.81745 | 583.45711 | 646.14392 | 712.48338 |
| 12  | 340.17804 | 382.31153 | 428.67350 | 479.46420 | 534.47640 | 597.63396 | 664.93438 | 735.20847 | 812.48338 |
| 13  | 401.16937 | 445.83785 | 495.36688 | 549.40007 | 603.45793 | 664.93438 | 735.20847 | 812.48338 | 897.20847 |
| 14  | 466.55550 | 514.28624 | 566.88206 | 624.40969 | 686.09616 | 748.46420 | 810.63396 | 882.48338 | 967.20847 |
| 15  | 536.87643 | 587.65804 | 649.36688 | 713.40007 | 776.45793 | 838.46420 | 900.43438 | 972.48338 | 1057.20847 |
| 16  | 612.13217 | 672.36339 | 731.70558 | 801.40007 | 876.45793 | 948.46420 | 1019.63396 | 1092.48338 | 1177.20847 |

8. Numerical results

The second derivatives $d_n = d^2\beta_n/dn^2$ of the asymptotic critical parameters (63) are presented in table 1 along with the values of $\Lambda_n,l = \beta_{n+1,l} - 2\beta_{n,l} + \beta_{n-1,l}$ which approximate the general second derivative $d^2\beta_n/dn^2$ numerically. It is seen that for the numerical second derivative $\Delta_n,l$, the speed $u_l$ of a convergence to the asymptotic value $d_l (l \to \infty)$ depends on the number of bound states $n$. The fastest convergence corresponds to the smallest $n = 1$. A similar situation is observed for the speed $u_n$ of the convergence of $\Lambda_n,l$ to $d_e (n \to \infty)$. In this case, the fastest convergence corresponds to the smallest $l = 0$.

Using the first and second methods described in sections 4 and 5, respectively, we have computed the critical parameters for a few widely used central potentials included in the nonrelativistic Schrödinger equation. The results for the exponential, Hulthen, Yukawa and Gaussian potentials are presented in tables 2–5, respectively. The critical parameters for the Woods–Saxon potential with $x_0 = 1$ and $x_0 = 0.001$ are exhibited in tables 6 and 7, respectively. The first value of the parameter $x_0$ presents the minimal value of the parameter $R = 0$ (see appendix A.4). By contrast, the second value of the parameter $x_0$ corresponds to the case of a large value of $R/r_0$ corresponding, e.g., to the optical-model calculations [20].
Table 3. Critical parameters $\beta = 2mg^2h^{-2}$ of the Hulthen potential $V(r) = -g \exp(-r/r_0)/(1 - \exp(-r/r_0))$.

| n \(\lambda\) | 0 | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 1 | 5.3059406 | 12.685368 | 23.146783 | 36.693671 | 53.327421 | 73.048651 | 95.857670 | 121.75465 |
| 2 | 4 | 10.724673 | 20.499398 | 33.348492 | 49.279726 | 68.296123 | 90.399036 | 115.58915 | 143.86682 |
| 3 | 9 | 18.100968 | 30.253614 | 45.480804 | 63.790287 | 85.185101 | 109.66659 | 137.23540 | 167.89189 |
| 4 | 16 | 27.448026 | 41.962702 | 59.557425 | 80.237830 | 104.90568 | 130.86162 | 160.80588 | 193.83855 |
| 5 | 25 | 38.775435 | 55.636363 | 75.588244 | 98.631880 | 124.76686 | 153.99258 | 186.30851 | 221.71423 |
| 6 | 36 | 52.086245 | 71.281353 | 93.580632 | 118.97988 | 147.47591 | 179.06647 | 213.74998 | 251.52532 |
| 7 | 49 | 67.384298 | 88.902568 | 113.54024 | 141.28775 | 172.13879 | 206.08916 | 243.13540 | 283.27733 |
| 8 | 64 | 84.671878 | 108.50368 | 135.47149 | 165.56029 | 198.76046 | 235.06562 | 274.47149 | 316.97510 |
| 9 | 81 | 103.95066 | 130.08753 | 159.37792 | 191.80146 | 227.34506 | 266.00010 | 307.70072 |           |
| 10 | 100 | 125.22192 | 153.65633 | 185.26240 | 220.01452 | 257.86913 | 298.89626 | 346.51175 |           |
| 11 | 121 | 148.48665 | 179.21189 | 213.12731 | 250.20224 | 290.41668 | 336.48500 | 392.39168 |           |
| 12 | 144 | 173.74563 | 206.75567 | 242.97402 | 282.36996 | 346.46731 | 391.79385 | 460.20943 |           |
| 13 | 169 | 200.99951 | 236.28888 | 274.80601 | 325.85339 | 391.46707 | 469.16916 | 559.95964 |           |
| 14 | 196 | 230.24882 | 267.81254 | 316.49349 | 381.39765 | 457.89073 | 546.46863 | 651.63620 |           |
| 15 | 225 | 261.49399 | 318.83000 | 381.37422 | 457.85666 | 547.22711 | 657.65669 | 775.23229 |           |
| 16 | 256 | 292.74418 | 351.98731 | 422.61373 | 507.23666 | 607.97145 | 727.81284 | 860.73696 |           |

The critical parameters for the exponential, Hulthen and Woods–Saxon potentials appearing in the Schrödinger equation with the orbital angular momentum quantum number $l = 0$ (S-states) can be calculated analytically. For the exponential and Woods–Saxon potentials, the requested solutions ($l = 0$) are proportional to the squares of zeros of the corresponding special functions (see the appendix). It is worth noting that the critical parameters for the Hulthen potential ($l = 0$) have an especially simple form. They are equal to $n^2$ where the number of bound states equals $n$. All these parameters are displayed in tables 2, 3, 6 and 7 for convenient comparison with the cases of $l > 0$. Note that the relative difference between the results obtained by the first method and the analytical ones is less than $10^{-14}$.

The critical parameters for the cut-off potential of the form (A.1) are not numerically presented here, because there is no problem to provide the proper calculations according to equation (A.7) for any orbital quantum number $l$ and parameter $s$. However, we have performed the corresponding computations in order to test both the first and second methods. The relative difference was less than $10^{-12}$ for the second method (section 5) for $l \leqslant 20$. The first method provides the same accuracy only for small values of $l \leqslant 3$, whereas for large $l$ this accuracy can be provided only for $l + n \leqslant 20$. One should note that all computations were performed...
Table 4. Critical parameters $\beta = 2m g r_0 \hbar^{-2}$ of the Yukawa potential $V(r) = -g \exp(-r/r_0)/r$.

| $n \setminus l$ | 0  | 1   | 2   | 3   | 4   | 5   | 6   | 7   | 8   |
|----------------|----|-----|-----|-----|-----|-----|-----|-----|-----|
| 1              | 1.6798078 | 9.0819590 | 21.891984 | 40.135552 | 63.808976 | 92.917164 | 127.46092 | 167.44064 | 212.85654 |
| 2              | 6.4472603 | 17.745576 | 34.240144 | 56.511114 | 84.036777 | 116.99234 | 155.38248 | 199.20797 | 248.46926 |
| 3              | 14.342028 | 29.461426 | 49.969576 | 75.899394 | 107.20637 | 144.05569 | 186.28566 | 233.95349 | 287.05673 |
| 4              | 25.371660 | 44.261254 | 68.571467 | 98.317925 | 133.50366 | 174.12875 | 220.19272 | 271.69505 | 328.63535 |
| 5              | 39.538442 | 62.160193 | 90.245270 | 123.78892 | 162.78498 | 207.22876 | 257.11705 | 312.44769 | 373.21919 |
| 6              | 56.84486  | 83.168247 | 115.60434 | 152.32675 | 195.11871 | 243.36968 | 297.07295 | 356.22417 | 420.82039 |
| 7              | 77.290455 | 107.29208 | 142.85836 | 183.94242 | 230.51632 | 282.56299 | 340.07168 | 403.03541 | 471.44949 |
| 8              | 100.87607 | 134.53636 | 173.81459 | 218.64457 | 268.97811 | 324.81824 | 386.12280 | 452.89086 | 525.11571 |
| 9              | 127.60202 | 164.90453 | 207.87862 | 256.44012 | 310.53874 | 370.13447 | 435.23449 | 505.79870 |               |
| 10             | 157.46853 | 198.39917 | 245.05485 | 297.33466 | 355.77058 | 418.45450 | 487.41381 | 545.31066 |               |
| 11             | 190.47575 | 235.02231 | 285.34681 | 341.33284 | 402.90900 | 470.03018 | 566.34038 | 609.8596   |               |
| 12             | 226.62381 | 274.77554 | 328.75740 | 388.43851 | 453.73757 | 528.17003 | 511.08099 | 439.40354 |               |
| 13             | 265.91281 | 317.66016 | 375.28899 | 438.65494 | 504.47915 | 573.08136 | 458.82871 | 491.01331 |               |
| 14             | 308.34282 | 363.67724 | 424.94360 | 493.12021 | 553.83444 | 478.98522 | 408.57254 | 345.59639 |               |
| 15             | 353.91391 | 412.82768 | 485.19765 | 567.31664 | 670.89760 | 549.86991 | 493.30010 | 393.16658 |               |
| 16             | 402.62614 | 482.98698 | 599.51605 | 521.48163 | 448.88371 | 381.72227 | 319.99729 | 263.70873 |               |

by means of the simplest Mathematica-7 codes using the standard (default) working precision. It is possible, of course, to enhance the calculation accuracy using, e.g., the better working precision.

Due to the lack of space, we have restricted the results in our tables to eight significant figures and values of $l + n \leq 16$.

The Yukawa potential is the only one for which we have revealed some earlier results on critical parameters [21]. They are presented there as the critical screening length for the one-electron eigenstates which were obtained in the frame of standard energy calculations. Those results are limited by five significant figures and $l + n \leq 9$, and coincide practically with those exhibited here in table 4.

For the Gaussian potential, we have found only the results of the binding energy calculations (see, e.g., [22–25]). These energies were computed for $l + n \leq 8$ and were completely consistent with the critical parameters presented here in table 5.

9. Conclusions

In conclusion, we would like to emphasize that the critical parameters are not of some particular character.
First, they present some universal characteristics of central potentials which possess the properties presented in equations (1)–(3).

Second, using the tables of these parameters, one can answer the following questions:

(1) What is the number $n$ of bound states for the given central potential and given orbital quantum number $l$?

(2) What is the maximum value of $l$ which can provide a bound state for the given central potential, or vice versa, what is the minimum critical parameter which can provide a bound state with a given $l$ for the given central potential?

(3) What is the mutual arrangement (order) of the energy levels $E_{n,l}$ (characterized by the quantum numbers $n$ and $l$) for the given form of central potential?

It is clear that the binding energy $E_{n,l}$ rises as the number $n$ of bound states or the orbital angular momentum quantum number $l$ increases. Tables 2–7 show that the critical parameters $\beta_{n,l}$ exhibit the same properties with respect to the numbers \{n, l\}. It is important to realize that for any two sets \{n₁, l₁\} and \{n₂, l₂\}, it follows from the inequality

$$\beta_{n₁,l₁} > \beta_{n₂,l₂}$$

for the given central potential that

$$E_{n₁,l₁} > E_{n₂,l₂}.$$
Table 6. Critical parameters $\beta = 2mg^2\alpha^2\hbar^{-2}$ of the Woods–Saxon potential $V(r) = -g/[1 + \exp(r/r_0)]$.

| n\l | 0   | 1   | 2   | 3   | 4   | 5   | 6   | 7   | 8   |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| 1   | 1.7205730 | 8.2135317 | 18.813940 | 33.542490 | 52.406813 | 75.410024 | 102.553558 | 133.83814 | 169.26419 |
| 2   | 9.6742198 | 20.755782 | 35.931282 | 55.231021 | 78.65326 | 106.23821 | 137.951407 | 242.396888 | 271.32232 |
| 3   | 23.969284 | 39.431300 | 59.073131 | 82.876856 | 109.83541 | 142.94481 | 179.2025315 | 219.60692 | 264.15685 |
| 4   | 44.615717 | 64.332441 | 88.346797 | 116.58590 | 149.01715 | 185.62315 | 226.3936688 | 271.32232 | 320.40492 |
| 5   | 71.64405 | 95.502170 | 123.81377 | 156.42640 | 193.28014 | 234.34169 | 279.5910515 | 329.01551 | 382.60663 |
| 6   | 104.96555 | 132.96409 | 165.51246 | 202.44471 | 243.67452 | 289.15197 | 338.8462258 | 392.73727 | 450.81159 |
| 7   | 144.66921 | 176.73264 | 213.46842 | 254.67366 | 300.23751 | 350.09364 | 404.2000074 | 462.52874 | 525.06071 |
| 8   | 190.72542 | 226.81735 | 267.69958 | 313.13737 | 362.99747 | 417.19781 | 475.6851818 | 538.42365 | 605.38815 |
| 9   | 243.13418 | 283.22488 | 328.21898 | 377.85407 | 431.97649 | 490.48934 | 553.3285074 | 620.44998 | 691.78238 |
| 10  | 301.89551 | 345.96008 | 395.03646 | 448.83786 | 507.19210 | 569.98836 | 637.1520405 | 591.78238 | 7 |
| 11  | 367.00940 | 415.02662 | 468.15961 | 526.09990 | 588.65845 | 655.71141 | 725.49305 | 558.22885 | 6 
| 12  | 438.47587 | 490.42734 | 547.59441 | 609.64918 | 676.38713 | 750.26737 | 833.7000406 | 646.52874 | 7 
| 13  | 516.29490 | 572.16450 | 633.34572 | 709.49305 | 758.22885 | 825.55183 | 914.21400 | 737.92737 | 8 
| 14  | 600.46650 | 660.23992 | 723.41749 | 798.79929 | 872.67311 | 965.69043 | 1065.90181 | 834.2365 | 9 
| 15  | 690.90668 | 754.65510 | 824.75901 | 905.91083 | 993.24081 | 1091.64093 | 1200.39154 | 932.85154 | 10 
| 16  | 787.86743 | 853.21997 | 926.80068 | 1008.52232 | 1106.38667 | 1217.39154 | 1338.31914 | 1043.81394 | 11 

Therefore, from the presented tables we can deduce the following important properties of the discrete energy spectrum of the considered central potentials:

$E_{n,l} > E_{n+1,l-1}$ for the Hulthen and Yukawa potentials,

$E_{n,l} < E_{n+1,l-1}$ for the exponential, Gaussian and Woods–Saxon potentials.

This probably relates to the fact that the Hulthen and the Yukawa potentials are singular at the origin.

It was established that the leading terms of the asymptotic expansions of the critical parameters $\beta_{n,l}$ have the following forms:

$$\beta_{n,l} \simeq \begin{cases} a_l l^2 & l \to \infty \\ a_n n^2 & n \to \infty \end{cases},$$  

where the general analytic expressions for the factors $a_l \equiv d_l/2$ and $a_n \equiv d_n/2$ are presented in section 7. The first of relationships (68) is valid for a finite number $n$ of bound states, whereas the second one is valid for a finite orbital angular momentum quantum number $l$. It is important to note that according to equations (61)–(64), both $a_l$ and $a_n$ are functions of the potential only (they do not depend on $l$ or $n$). The subscripts $l$ and $n$ in $a_l$ and $a_n$ reflect the only fact that $a_l$ corresponds to the coefficient of $l^2$ ($l \to \infty$), whereas $a_n$ corresponds to the coefficient of $n^2$ ($n \to \infty$).
Table 7. Critical parameters $\beta = 2mg^2R^2\hbar^{-2}$ of the Woods–Saxon potential $V(r) = -g/[1 + 0.001 \exp(r/R)]$

| n/ | 0  | 1  | 2  | 3  | 4  | 5  | 6  | 7  | 8  |
|----|----|----|----|----|----|----|----|----|----|
| 1  | 0.0514391 | 0.2136959 | 0.45411555 | 0.77426459 | 1.1724439 | 1.6484948 | 2.2023382 | 2.8339302 | 3.5432443 |
| 2  | 0.4052507 | 0.7463148 | 1.16530509 | 1.66173344 | 2.2359950 | 2.8880871 | 3.6179882 | 4.4256753 | 5.3111276 |
| 3  | 1.0529125 | 1.5655339 | 2.15833822 | 2.8284741 | 3.5768555 | 4.4034793 | 5.3081665 | 6.2908725 | 7.3515353 |
| 4  | 1.9863174 | 2.6709161 | 3.4345909 | 4.2773825 | 5.1986738 | 6.1987162 | 7.272089 | 8.4340224 | 9.6690512 |
| 5  | 3.206640 | 4.0606118 | 4.9951932 | 6.0094520 | 7.103599 | 8.2753888 | 9.5272608 | 10.857441 | 12.266128 |
| 6  | 4.7125157 | 5.7361307 | 6.8408115 | 8.0259370 | 9.290171 | 10.635665 | 12.059576 | 13.562505 | 15.144255 |
| 7  | 6.5057952 | 7.6977523 | 8.9718549 | 10.327215 | 11.763171 | 13.279221 | 14.874975 | 16.550125 | 18.304425 |
| 8  | 8.5859457 | 9.9456459 | 11.388595 | 12.913644 | 14.519959 | 16.206914 | 17.974033 | 19.829942 | 21.747345 |
| 9  | 10.95285 | 12.479924 | 14.091224 | 15.785486 | 17.561701 | 19.419123 | 21.357183 | 23.375440 | 25.523478 |
| 10 | 13.60692 | 15.300668 | 17.079885 | 18.942937 | 20.888645 | 22.916139 | 25.024758 | 27.137676 | 29.403429 |
| 11 | 16.547758 | 18.407936 | 20.354690 | 22.386154 | 24.509987 | 26.698194 | 28.97559 | 31.383051 | 33.884056 |
| 12 | 19.775499 | 21.801777 | 23.915725 | 26.115262 | 28.398884 | 30.962114 | 33.618555 | 36.458804 | 39.488932 |
| 13 | 23.290146 | 25.482228 | 27.763062 | 30.130362 | 32.589823 | 35.182647 | 37.834271 | 40.642209 | 43.514326 |
| 14 | 27.091699 | 29.449318 | 31.896761 | 34.487777 | 37.27904 | 40.090819 | 43.065447 | 46.190460 | 49.398006 |
| 15 | 31.180159 | 33.703074 | 36.256127 | 38.904356 | 41.630284 | 44.391655 | 47.215216 | 50.129872 | 53.125861 |
| 16 | 35.555527 | 38.087331 | 40.606340 | 43.252072 | 45.975311 | 48.737346 | 51.549761 | 54.430263 | 57.384776 |

Summing up, we would like to stress that the highest excited bound state of a potential with critical parameter $\beta_c$ is a transition state. The parameter $\beta_c$ presents an exact numerical value, and the transition state corresponds to a fictitious (threshold) state with energy $E(\beta_c) = 0$. In practice, it is impossible to calculate $\beta_c$ to absolute accuracy, and the transition state can be seen as emerging from the limit bound state with an arbitrarily small binding energy.

The physical significance of the transition states is not limited to the questions addressed in this work. It is easy to show that infinite scattering lengths correspond to transition $S$-states. The so-called Fano–Feshbach resonance, for example, as well as many other physical effects, are characterized, in turn, by such infinite scattering length (see, e.g., [29] and references therein).

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Appendix

A.1. Finite square well-like potential

Let us examine potential of the form

\[ V(r) = \begin{cases} \frac{g}{r^s}, & r \leq r_0 \\ 0, & r > r_0 \end{cases} \quad (s < 2). \quad (A.1) \]

For \( s = 0 \), one obtains the potential which is widely known as the finite square well. Equation (9) with the potential (A.1) reduces to the form

\[ \chi''(r) = \left[ -\frac{\beta}{r^s} H(1 - r) + \frac{l(l+1)}{r^2} \right] \chi(r), \quad (A.2) \]

where \( H(x) \) is the Heaviside step function. The parameter \( \beta \) is defined by equation (12). A particular solution satisfying the asymptotic condition (20) and vanishing at the origin has a form

\[ \chi(r) = \begin{cases} A \sqrt{r} J_\alpha \left( \frac{\sqrt{\beta}}{r} \right), & r \leq 1 \\ Br^{-l}, & r > 1 \end{cases} \quad (A.3) \]

with \( \nu = \frac{2 - s}{2}, \quad \alpha = \frac{2l + 1}{2 - s}. \quad (A.4) \)

Here \( J_\nu(z) \) is the Bessel function of the first kind, whereas \( A \) and \( B \) are arbitrary constants.

Matching the logarithmic derivatives of solutions (A.3) at the point \( r = 1 \), one obtains the following equation for \( \beta \):

\[ \sqrt{\beta} \left[ (l+1)J_{\nu-1} \left( \frac{\sqrt{\beta}}{\nu} \right) - \nu J_{\nu+1} \left( \frac{\sqrt{\beta}}{\nu} \right) \right] = -l(2l+1)J_{\nu} \left( \frac{\sqrt{\beta}}{\nu} \right). \quad (A.5) \]

Using the properties of the Bessel functions [15], one can reduce equation (A.5) to the following simplest equation:

\[ J_{2\nu+1} \left( \frac{2\sqrt{\beta}}{2-s} \right) = 0. \quad (A.6) \]

The explicit solution of equation (A.6) has a form

\[ \beta_n \equiv \left[ \frac{2-s}{2} j_{2\nu+n} \right]^2 \quad (n = 1, 2, \ldots), \quad (A.7) \]

where \( j_{\mu,n} \) presents the \( n \)th positive zero of the Bessel function \( J_\mu(z) \).

From expansion (9.5.12) [15] for large zeros, one has

\[ j_{\nu,n} \simeq \left( n + \frac{\nu}{2} - \frac{1}{4} \right) \pi - \frac{4\nu^2 - 1}{8 (n + \nu - \frac{1}{2}) \pi} = \frac{4(4\nu^2 - 1)(28\nu^2 - 31)}{192 (n + \nu - \frac{1}{2})^3 \pi^3} - \cdots . \quad (A.8) \]

Putting \( \nu \equiv \nu_{\nu,s} = \frac{2}{2-s} - \frac{1-s}{2-s} \),

\[ \beta_n \sim (\frac{2-s}{2})^2 \pi^2 n^2. \quad (A.9) \]
This yields, in particular,
\[ \frac{d^2}{dn^2} \beta_n(s = 0) \simeq \frac{2\pi^2}{2n^2}, \quad \frac{d^2}{dn^2} \beta_n(s = 1) \simeq \frac{\pi^2}{2n^2}. \]  
(A.11)

From expansion for zeros of the Bessel functions of large order [26] (see, also (9.5.14) [15]), one has
\[ j_{\nu, n} = \nu \left( 1 + \sum_{k=1}^{\infty} \alpha_{k,n} \nu^{-\frac{2}{p}} \right). \]  
(A.12)

The first coefficients \( \alpha_{k,n} \) for \( \{k, n\} \leq 5 \) can be found in [26]. Thus, using equation (A.9), one obtains for large enough \( l \)
\[ \beta_n \equiv \beta_{n,l} = \left( l - \frac{1 - s}{2} \right)^2 \left[ 1 + \sum_{k=1}^{\infty} \alpha_{k,n} \left( \frac{2l - 1 + s}{2 - s} \right)^{-\frac{2}{p}} \right]^2. \]  
(A.13)

It is seen that the leading term of the asymptotic \( (l \to \infty) \) expansion of the critical parameter is given by
\[ \beta_{n,l} \to \frac{l^2}{\infty}. \]  
(A.14)

A.2. Exponential potential

The exponential potential has a form
\[ V(r) = -g \exp \left( -\frac{r}{r_0} \right). \]  
(A.15)

Equation (9) with the potential (A.15) reads
\[ \chi''(r) = \left[ -\beta \exp(-r) + \frac{l(l+1)}{r^2} \right] \chi(r). \]  
(A.16)

The parameter \( \beta \) is defined here by equation (12) with \( s = 0 \). Equation (A.16) has an analytical solution only for the case of \( l = 0 \). Such a particular solution satisfying the boundary condition (15) has a form
\[ \chi(r) = A \left[ J_0(q)Y_0(q e^{-r}) - Y_0(q)J_0(q e^{-r}) \right], \]  
(A.17)

where \( q = 2\sqrt{\beta} \), whereas \( J_0(z) \) and \( Y_0(z) \) are the Bessel functions of the first and second kind, respectively. The argument of the Bessel functions in equation (A.17) achieves zero as \( r \to \infty \). Therefore, using series expansion for the Bessel functions [15]
\[ J_0(q e^{-r}) \simeq \frac{q^2}{4} e^{-r}, \quad Y_0(q e^{-r}) \simeq -\frac{r}{\pi}, \]  
(A.18)

one should put
\[ J_0(q) = 0, \]  
(A.19)

in order that solution (A.17) satisfies the asymptotic boundary condition (20). Taking into account condition (A.19) for the transition state, and the first of expansions (A.18), one can write for the asymptotic behavior of the solution (A.17)
\[ \chi(r) \simeq -\frac{r}{\pi} J_0(2\sqrt{\beta})(1 - \beta e^{-r}). \]  
(A.20)

From equation (A.19), one obtains for the critical parameters
\[ \beta_n = \frac{j_{0,n}^2}{4}, \quad (n = 1, 2, \ldots), \]  
(A.21)

where \( j_{0,n} \) presents the \( n \)th positive zero of the Bessel function \( J_0(z) \).
Putting $\nu = 0$ in expansion (A.8) for large zeros, one obtains
\[ j_{0,n} \simeq \left( n - \frac{1}{4} \right) \pi + \frac{1}{2(4n - 1)\pi} - \frac{124}{3(4n - 1)^3\pi^3} + \cdots. \] (A.22)

This yields
\[ \beta_n \simeq \frac{\pi^2}{4} \left( n - \frac{1}{4} \right)^2. \] (A.23)

The value of second derivative $\lim_{n \to \infty} \frac{d^2 \beta_n}{dn^2} = \pi^2/2$ coincides with the corresponding value (A.11) for the FSW-like potential with $s = 1$.

### A.3. Hulthen potential

For the Hulthen potential
\[ V(r) = -g e^{-r/r_0} - e^{-r/r_0}, \] (A.24)
equation (9) becomes
\[ \chi''(r) = \left[ -\frac{\beta}{e^r - 1} + \frac{l(l+1)}{r^2} \right] \chi(r). \] (A.25)

For this differential equation, one can obtain a general analytic solution of the form
\[ \chi(r) \equiv \phi(x) = Ax^{-\alpha} {}_2F_1(-\alpha, -\alpha; 1 - 2\alpha; x) + Bx^\alpha {}_2F_1(\alpha, \alpha; 1 + 2\alpha; x) \] (A.26)
with
\[ \alpha = \sqrt{\beta}, \quad x = e^r, \] (A.27)
only for $S$-states ($l = 0$). Here $_2F_1(a; b; c; z)$ is the Gauss hypergeometric function, and $A$ and $B$ are arbitrary constants.

Formulas (15.1.20) and (6.1.18) [15] yield
\[ _2F_1(a; a; 1 + 2a; 1) = \frac{4^{\alpha} \Gamma(a + 1/2)}{\sqrt{\pi} \Gamma(a + 1)}, \] (A.28)

where $\Gamma(z)$ denotes Euler’s gamma function. The latter representation enables us to obtain the vanishing at the origin ($r \to 0 \Rightarrow x \to 1$) solution in the form
\[ \chi(r) \equiv \varphi(x) = C \left[ \left( \frac{x}{4} \right)^{\alpha} \Gamma(1 - \alpha) \Gamma \left( \frac{1}{2} + \alpha \right) {}_2F_1(-\alpha, -\alpha; 1 - 2\alpha; x) - \left( \frac{x}{4} \right)^{-\alpha} \Gamma(1 + \alpha) \Gamma \left( \frac{1}{2} - \alpha \right) {}_2F_1(\alpha, \alpha; 1 + 2\alpha; x) \right], \] (A.29)
with arbitrary constant $C$. For the examination of the asymptotic behavior of solution (A.29), one can use formula (15.3.13)[15], which yields
\[ (-x)^a _2F_1(a, a; 1 + 2a; x) \simeq \frac{2 \Gamma(2a)}{\Gamma^2(a)} \ln(-x). \] (A.30)

Inserting the asymptotic representation (A.30) for $a = \alpha$ and $a = -\alpha$ into the rhs of equation (A.29), one obtains after some transformations
\[ \chi(r) \simeq -2Ca \sqrt{\pi} (\pi r + r) \] (A.31)
on the other hand, the series expansion of solution (A.29) near $x = 1$ ($r \to 0$) yields
\[ \chi(r) \simeq -2Ca^2 \pi^{3/2} \csc(\pi \alpha) r. \] (A.32)
Putting
\[ C = - [2\alpha^2 \pi^{3/2} \csc(\pi \alpha)]^{-1}, \]  
(A.33)
one can get rid of \( \alpha \)-dependence for the leading term of the \( \chi (r) \) series expansion. Substituting
expression (A.33) into the asymptotic representation (A.31), one finally obtains
\[ \chi (r) \simeq \frac{\sin(\pi \alpha)}{\pi \alpha} (i\pi + r). \]  
(A.34)
Thus, in order to satisfy asymptotic condition (20), one should put
\[ \sin(\pi \alpha) = 0 \quad (\alpha \neq 0). \]  
(A.35)
The roots of equation (A.35) are the integers, that is, \( \alpha_n = n \). Thus, from definition (A.27), one obtains that the critical parameters for the Hulthen potential can be determined from the simplest relation
\[ \frac{2mgy_0^2}{\hbar^2} = n^2 \quad (n = 1, 2, \ldots), \]  
(A.36)
where \( n \) is a number of \( S \)-bound states.

A.4. Woods–Saxon potential
Finally, let us examine the Woods–Saxon potential
\[ V (r) = - \frac{g}{1 + \exp \left( \frac{r - R}{r_0} \right)} \quad (R > 0), \]  
(A.37)
which is the most complicated one. For this case, equation (9) takes a form
\[ \chi''(r) = \left[ -\frac{\beta}{1 + x_0 e^r} + \frac{l(l + 1)}{r^2} \right] \chi (r), \]  
(A.38)
where \( \beta \) is defined by equation (12) with \( s = 0 \), whereas \( x_0 = \exp(-R/r_0) \). Equation (A.38) admits the analytical solution only for the case of \( l = 0 \). Introducing a new variable \( x = x_0 e^r \) and a new parameter \( \alpha = \sqrt{\beta} \), one obtains a new differential equation
\[ x^2 \psi''(x) + x \psi'(x) + \frac{\alpha^2}{1 + x} \psi(x) = 0 \]  
(A.39)
for the function \( \psi(x) \equiv \chi (r) \). The vanishing at the origin solution of equation (A.39) has a form
\[ \psi(x) = C \left[ F(-\alpha, x_0) F(\alpha, x) - F(\alpha, x_0) F(-\alpha, x) \right], \]  
(A.40)
where
\[ F(\alpha, x) = x^\alpha \mathbb{F}_1(i\alpha, i\alpha; 1 + 2i\alpha; -x). \]  
(A.41)
Here \( \mathbb{F}_1(a, b; c; z) \) is the Gauss hypergeometric function and \( C \) is arbitrary constant. For the considered case, formula (15.3.13) \[15\] yields
\[ (x)^b \mathbb{F}_1(b, b + 1; -x) \simeq \frac{2\Gamma(2b)}{\Gamma^2(b)} \ln(x). \]  
(A.42)
Inserting the latter representation into solution (A.40) and returning to the initial variable \( r \), one obtains
\[ \chi (r) \simeq 2C(r + \ln x_0) \left[ \frac{F(-\alpha, x_0) \Gamma(2i\alpha)}{\Gamma^2(i\alpha)} - \frac{F(\alpha, x_0) \Gamma(-2i\alpha)}{\Gamma^2(-i\alpha)} \right] \]  
\[ = 2C(r + \ln x_0) i\alpha \mathbb{F}_1 \left( -i\alpha, i\alpha; 1; -\frac{1}{x_0} \right). \]  
(A.43)
Thus, to satisfy condition (20) for the transitional states, one should put

$$2F_1 \left( -i\alpha, i\alpha; 1; -\frac{1}{x_0} \right) = 0.$$  \hspace{1cm} (A.44)

The roots $\beta_n = \alpha_n^2$ of the latter transcendental equation present the desired critical parameters for a given $x_0$. It is worth noting that equation (A.44) can be simplified if one uses the following relationships between the Gauss hypergeometric functions, the Jacobi functions $P_{\nu}^{(a,b)}$ and the Legendre functions $P_{\nu}$:

$$2F_1 \left( -i\alpha, i\alpha; 1; -z \right) = P_{\nu}^{(0,-1)} (2z + 1) = (1 + z) P_{\nu}^{(0,1)} (2z + 1) = \text{Re} \left[ P_{\nu} (2z + 1) \right]$$

$(\alpha > 0, \ z > 0)$.

(A.45)

According to the asymptotic expansion for the Legendre function of imaginary degree (see equation (3.2), [27]), one has

$$\text{Re} \left[ P_{\nu} (\cosh t) \right] \simeq \frac{1}{\sqrt{2}} \sum_{k=0}^{N} (2k - 1)!a_k(t) \left( -\frac{t}{\alpha} \right)^k J_k(\alpha t) + O(\alpha^{-N-1}),$$

where

$$a_0(t) = \sqrt{t \coth \left( \frac{t}{2} \right)}, \quad a_1(t) = \frac{a_0(t)}{8t} \left( \frac{\cosh t - 2}{\sinh t} + \frac{1}{t} \right).$$  \hspace{1cm} (A.47)

In zero approximation for large enough $\alpha$, one can put $N = 0$, whence

$$\text{Re} \left[ P_{\nu} (\cosh t) \right] \underset{\alpha \to \infty}{\simeq} \frac{1}{\sqrt{2}} \sqrt{t \coth \left( \frac{t}{2} \right)} J_0(\alpha t).$$  \hspace{1cm} (A.48)

Thus, roots of equation (A.44) for large enough $\alpha = \sqrt{\beta}$ are very close to zeros of the Bessel function $J_0(\alpha t)$, where

$$t = \arccosh \left( \frac{2}{x_0} + 1 \right) = 2 \arcsinh \left( \frac{1}{\sqrt{x_0}} \right) = 2 \ln \left( \frac{1 + \sqrt{x_0} + 1}{\sqrt{x_0}} \right).$$

(A.49)

In terms of zeros $j_{0,n}$ of the Bessel functions, one can then write down

$$j_{0,n} \simeq 2 \sqrt{\beta} \ln \left( \frac{1 + \sqrt{x_0} + 1}{\sqrt{x_0}} \right).$$

(A.50)

Taking into account expansion (A.22), one finally obtains

$$\beta_n \underset{n \to \infty}{\simeq} \frac{\pi^2}{4 \ln^2 \left( \frac{1 + \sqrt{x_0} + 1}{\sqrt{x_0}} \right)} \left( n - \frac{1}{4} \right)^2.$$  \hspace{1cm} (A.51)

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