Application of the Fröbenius method to the Schrödinger equation for a spherically symmetric potential: anharmonic oscillator

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Abstract.
The power series method has been adapted to compute the spectrum of the Schrödinger equation for central potential of the form \( V(r) = \frac{d}{r^2} + \frac{d-2}{r} + \sum_{i=0}^{\infty} d_i r^i \). The bound-state energies are given as zeros of a calculable function, if the potential is confined in a spherical box. For an unconfined potential the interval bounding the energy eigenvalues can be determined in a similar way with an arbitrarily chosen precision. The very accurate results for various spherically symmetric anharmonic potentials are presented.
1. Introduction

The exact solution of the Schrödinger equation can be obtained only for a few particular forms of potentials, in other cases one has to resort to approximations or numerical techniques. Many approximation methods have been developed for solving problems in one-dimensional space. Approximate solutions to the Schrödinger equation have been also studied for spherically symmetric potentials in $D$-dimensional space, both by methods elaborated for one-dimensional space, e.g. the Hill determinant method [1], the variational approach [2], and by methods dedicated to D-dimensional problems, e.g. the shifted 1/D expansion [3, 4]. Here we show that highly accurate solutions to the Schrödinger equation can be determined for various types of spherically symmetric potentials with the use of the Fröbenius method (FM). The method consists in expanding the solution of a differential equation into power series [5], and was originally applied by Barakat and Rosner [6] to compute the spectrum of one-dimensional quartic oscillator confined by impenetrable walls at $x = \pm R$. The energy eigenvalues of the system have been obtained numerically as zeros of a function, calculated from its power series representation. Moreover, it has been shown that the bound-state energies of the confined system approach rapidly those of the unconfined oscillator for increasing $R$. Low-lying eigenvalues for other one-dimensional potentials [7] have been also successfully calculated in a similar way. Recently, a modified treatment of unconfined systems allowed for a very accurate determination of the ground-state energy for the quartic oscillator [8]. In all the cases studied the potential was a finite function, and a solution was expanded around an ordinary point of the differential equation. Here we study the application of the FM for solving the radial Schrödinger equation, which requires that an expansion around a regular singular point should be used.

The outline of the present work is as follows. In Section 2 the solution of the radial Schrödinger equation in form of a generalized power series is discussed. The case of a spherically symmetric potential bounded by an impenetrable wall at $r = R$ is studied in Section 3. In this case, the energy eigenvalues can be easily determined by finding the roots of the polynomial, which is illustrated on the example of the confined harmonic and anharmonic oscillators and Hulthén potential. The case of unconfined system is studied in Section 4 where a scheme for determining an arbitrarily large set of bound-state energies is developed. After demonstrating the performance of the method on the exactly solvable example of the Kratzer potential, the results for the unconfined oscillator are presented for various choices of anharmonic parameters.

2. Expansion around a regular-singular point

The Schrödinger equation for a spherically symmetric potential in 3-dimensional space can be reduced to an ordinary differential equation in the radial variable

$$\left[ -\frac{1}{2r} \frac{d^2}{dr^2} + \frac{l(l+1)}{2r^2} + V(r) \right] R(r) = \lambda R(r), \quad (1)$$
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where \( l \) is the angular momentum quantum number, and the units \( \hbar = 1, \ m = 1 \) are used. Upon introducing the function \( u(r) = rR(r) \), the differential equation (1) takes the form of the one-dimensional Schrödinger eigenvalue problem

\[
\left[ -\frac{1}{2} \frac{d^2}{dr^2} + V_{\text{eff}}(r, l) \right] u(r) = \lambda u(r),
\]  

(2)

where the effective potential reads

\[
V_{\text{eff}}(r, l) = \frac{l(l+1)}{2r^2} + V(r).
\]  

(3)

The point \( r = 0 \) is a regular singular point of the radial equation, if the potential \( V(r) \) diverges but \( r^2 V(r) \) remains finite as \( r \to 0 \), which is the case for the interaction potential of the form

\[
V(r) = \frac{d}{r^2} + \frac{d_{-1}}{r} + V_{\text{reg}}(r),
\]  

(4)

where the regular part is represented by a convergent series

\[
V_{\text{reg}}(r) = \sum_{i=0}^{\infty} d_i r^i.
\]  

(5)

In this case the FM can be applied with the radial wave function represented as a generalized power series

\[
u(r) = r^\delta \sum_{i=0}^{\infty} a_i r^i,
\]  

(6)

where \( a_0 \neq 0 \). In what follows, we will take \( a_0 = 1 \), since normalization of wave function is irrelevant in our calculation. Substituting (6) into (2) we obtain the equation

\[
-\frac{1}{2} \sum_{i=0}^{\infty} \left[ (i+\delta)(i+\delta-1) - l(l+1) \right] a_i r^i + \left( \sum_{i=0}^{\infty} d_{i-2} r^i \right) \left( \sum_{i=0}^{\infty} a_i r^i \right) = \lambda \sum_{i=0}^{\infty} a_i r^{i+2},
\]  

(7)

which, by comparing the coefficients of like powers of \( r \), yields the recurrence relation

\[
[(i + \delta)(i + \delta - 1) - l(l+1)] a_i - 2 \sum_{n=0}^{i} d_{i-2-n} a_n + 2a_{i-2} \lambda = 0,
\]  

(8)

where \( a_i = 0 \) for \( i < 0 \). Setting \( i = 0 \) in the above relation, we obtain the indicial equation

\[
[\delta(\delta - 1) - l(l+1) - 2d_{-2}] a_0 = 0,
\]  

(9)

which is solved by

\[
\delta_1 = \frac{1}{2} \left( 1 - \sqrt{8d_{-2} + (1 + 2l)^2} \right), \quad \delta_2 = \frac{1}{2} \left( 1 + \sqrt{8d_{-2} + (1 + 2l)^2} \right).
\]  

(10)

The Fuchs’s theorem \([5]\) asserts that the generalized series (6) converges, and both linearly independent solutions of the Schrödinger equation (2) are obtained as generalized series, one with \( \delta = \delta_1 \) and the other with \( \delta = \delta_2 \) (except the special case when \( \delta_2 - \delta_1 = \sqrt{8d_{-2} + (1 + 2l)^2} \) is equal to a non-negative integer). The value of \( \delta \) determines the behavior of \( u(r) \) for \( r \to 0 \), and only \( \delta > \frac{1}{2} \) is acceptable \([9]\), since only in this case the mean value of the kinetic energy is finite. Such a solution to the Schrödinger
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Equation (2) exists only if the potential is such that \( d_{-2} > -\frac{1}{8} \). This solution contains only the series with \( \delta = \delta_2 \), and in the following will be denoted by

\[
u(r, \lambda) = r^{\delta_2} \sum_{i=0}^{\infty} a_i r^i,
\]

where the dependence on the energy eigenvalue \( \lambda \) is explicitly marked. The coefficients of the series are determined recurrently as

\[
a_i = \frac{-2\lambda a_{i-2} + 2 \sum_{n=0}^{i-1} d_{i-2-n} a_n}{i(i + \sqrt{8d_{-2} + (1 + 2l)^2})}.
\]

The function \( u(r, \lambda) \) has an important property that \( u(0, \lambda) = 0 \), which can be regarded as a boundary condition for the radial equation at \( r = 0 \). The second boundary condition should be chosen according to the physical bounds in the investigated problem.

3. Confined potentials

The simplest scheme arises in case of radially symmetric potential \( V(r) \) additionally bounded by an infinitely high wall at \( r = R \). In this case the second boundary condition for a particle with angular momentum \( l \) is of the form

\[
u(R, \lambda) = 0,
\]

yielding an exact quantization condition that gives the bound state energies as zeros of a calculable function. The values of \( \lambda \), determined from the above condition, are will be denoted by \( \lambda_{nl} \), where \( n = 0, 1, \ldots \) counts the number of zeros in the radial variable in the Sturm-Liouville eigenvalue problem \[10\]. In the numerical calculation, the function \( u(R, \lambda) \) has to be approximated by truncating the series in \[11\] at suitably high order \( K \), which can be done with an arbitrary accuracy, as the series is convergent. The truncated function is a polynomial of degree \( K \) in the variable \( \lambda \), that can be used to advantage in determining the numerical values of its zeros. In this way an increasing amount of bound-state energies can be obtained with increasing accuracy as the truncation order \( K \rightarrow \infty \). Considering the growing interest in quantum confined systems, the method (and its possible modifications for different symmetries of the confining box) can find application in the studies of semiconductor nanostructures such as quantum dots \[11, 12, 13\]. Here we consider a few examples.

3.1. Harmonic Oscillator

The performance of the FM will be demonstrated for the spherical harmonic oscillator

\[
V(r) = \frac{\omega^2}{2} r^2,
\]

enclosed by a sphere of the radius \( R \). The typical behavior of \( u(R, \lambda) \) as a function of \( \lambda \) is shown in Fig.1 in the example of the oscillator with \( \omega = 1 \) for \( l = 0 \) and \( R = 2.5 \). The approximate \( u(R, \lambda) \) is a polynomial in \( \lambda \) and the truncation affects only its behavior for large \( \lambda \). We determine thus the bound state energies as roots of the
obtained polynomial with the use of NSolve procedure from the Mathematica package, without any need for introducing starting values for $\lambda$. The stability of the numerical results was achieved by increasing the number of non-vanishing terms $K$ until the values of $\lambda_{nl}(R)$, corresponding to the states $(n, l)$ of angular momentum $l$, become stable to the desired accuracy. The values of $\lambda_{nl}(R)$, obtained for the harmonic oscillator of frequency $\omega = 1$, are compared in Table 1 with the eigenvalues of the unconfined oscillator, $E_{nl} = 2n + l + \frac{3}{2}$. In Fig. 2 the low-lying states energies are plotted as a function of the confinement radius $R$. One can observe how the non-degenerate levels of the confined system approach the equidistant states of the unconfined oscillator, as the radius of enclosure grows.

![Figure 1](image_url)  

**Figure 1.** Behavior of $u(R, \lambda)$ for the spherically symmetric harmonic oscillator with $\omega = 1$ and $l = 0$ at $R = 2.5$.

| $l$ | $n$ | $\lambda_{nl}(1.5)$ | $\lambda_{nl}(2.5)$ | $\lambda_{nl}(3)$ | $\lambda_{nl}(3.5)$ | $\lambda_{nl}(4)$ | $E_{nl}$ |
|-----|-----|---------------------|---------------------|------------------|------------------|------------------|--------|
| 0   | 0   | 2.5049762           | 1.5514217           | 1.5060815        | 1.5003995        | 1.5000146        | 1.5    |
| 1   | 0   | 4.9035904           | 2.6881440           | 2.5312925        | 2.5029102        | 2.5001438        | 2.5    |
| 0   | 1   | 9.1354221           | 4.1842613           | 3.6642196        | 3.5233023        | 3.5016915        | 3.5    |
| 2   | 0   | 7.8717305           | 3.9535289           | 3.5982477        | 3.5125803        | 3.5008421        | 3.5    |

### 3.2. Anharmonic Oscillator

The quantum anharmonic oscillator is widely used to describe the physical phenomena, especially in the condensed matter and molecular physics. However, the case of
a confined anharmonic system has been discussed only for the one-dimensional example [6]. Here we study the spherically symmetric anharmonic oscillator with a potential of the form

\[ V_{AO}(r) = \frac{\omega^2}{2} r^2 + g r^{2J} \]  

(15)

for different values of the power \( J \). The analysis can be simplified by using the rescaled variables

\[ \hat{r} = g^{\frac{1}{2J+1}} r, \quad \text{and} \quad \hat{\lambda} = \lambda g^{\frac{2}{2J+1}} \]

then Eq.(2) takes a form

\[ \left[ -\frac{1}{2} \frac{d^2}{d\hat{r}^2} + \frac{l(l+1)}{2\hat{r}^2} + V_{AO}(\hat{r}) \right] u(\hat{r}) = \hat{\lambda} u(\hat{r}), \]

(16)

where

\[ V_{AO}(\hat{r}) = z\hat{r}^2 + \hat{r}^{2J} \]

(17)

depends on the dimensionless parameter

\[ z = \frac{\omega^2}{2} g^{\frac{4}{2J+1}}, \]

(18)

which accounts for a relative strength of the harmonicity and anharmonicity. In the following, we skip the hats over \( r \) and \( \lambda \). We consider the solution of (16), which is regular at \( r = 0 \), as given by the generalized power series

\[ u(r, \lambda) = r^{l+1} \sum_{i=0}^{\infty} a_i r^{2i} \]

(19)

with the recurrence relation of the form

\[ a_i = \frac{-2\lambda a_{i-1} + 2za_{i-2} + 2a_{i-(J+1)}}{2i(1+2i+2l)}, \]

(20)

**Figure 2.** Behavior of \( \lambda_{nl}(R) - \lambda_{00}(R) \) for the harmonic oscillator in function of the confinement radius \( R \).
where \( a_0 = 1 \). In the case of the oscillator enclosed by a sphere of the radius \( R \) the bound-state energies are easily determined as zeros of \( u(R, \lambda) \). In Table 2 the numerical results are presented on the example of the quartic oscillator \((J = 2)\) with different values of the parameter \( z \) and for different radii of enclosure \( R \). The spectrum of an unconfined anharmonic oscillator will be studied in the next section.

### Table 2. The bound-state energies \( \lambda_{nl}(R) \) of the confined anharmonic oscillator

| \( l \) | \( n \) | \( z \) | \( \lambda_{nl}(0.5) \) | \( \lambda_{nl}(1) \) | \( \lambda_{nl}(1.5) \) | \( \lambda_{nl}(2) \) | \( \lambda_{nl}(2.5) \) |
|---|---|---|---|---|---|---|---|
| 0 | 0 | 5 | 20.09875027 | 6.39291817 | 5.10864245 | 5.06974045 | 5.06966368 |
| 4 | 20.02840681 | 6.13228781 | 4.69129108 | 4.63348473 | 4.63330831 |
| 3 | 19.95799389 | 5.86753935 | 4.24715028 | 4.16026790 | 4.15984713 |
| -1 | 19.67564622 | 4.76592159 | 2.12668280 | 1.63322595 | 1.61278177 |
| -3 | 19.53405395 | 4.18860246 | 0.80447958 | -0.38394286 | -0.54059117 |
| 1 | 40.85989845 | 12.08775101 | 8.80212012 | 8.63744701 | 8.63688371 |
| 4 | 40.76648791 | 11.73035216 | 8.1648083 | 7.93950715 | 7.9383601 |
| 3 | 40.67302607 | 11.36972235 | 7.49829458 | 7.18963353 | 7.18714592 |
| -1 | 40.29866554 | 9.89468226 | 4.51245222 | 3.40693967 | 3.34739553 |
| -3 | 40.11117731 | 9.13754642 | 2.81077229 | 0.78285838 | 0.50413322 |

#### 3.3. Hulthén potential

The FM can be also useful for computing energy eigenvalues, in case when the series expansion of its regular part (5) converges only in a finite interval \( \rho_V \). In this case, the convergence of the generalized series solution (11) is granted only for \( r < \rho_V \) and the problem is well defined only for the confinement radius \( R < \rho_V \). If the confining box projects beyond the convergence sphere, we must be very careful, since for \( r > \rho_V \) the series representation \( u(r, \lambda) \) does not necessarily coincide with the solution of the radial Schrödinger equation in the potential \( V(r) \). As an example, we consider the Hulthén potential

\[
V(r) = \frac{-\delta e^{-\delta r}}{1 - e^{-\delta r}},
\]

when the screening parameter \( \delta > 0 \) is not too large. To employ the FM we expand the Hulthén potential into the Laurent series

\[
V(r) = -\frac{1}{r} + V_{reg}(r),
\]

with the regular part given by

\[
V_{reg}(r) = \frac{\delta}{2} - \delta \sum_{n=0}^{\infty} g_n[\delta r]^{2n+1},
\]
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where

\[ g_n = \frac{(-1)^n \beta_{n+1}}{[2(n + 1)]!}, \quad (24) \]

and \( \beta_n \) are given \[14\] by a convenient expression

\[ \beta_n = (-1)^n \frac{n}{2^{2n} - 1} \sum_{k=1}^{2n-1} \frac{\sum_{j=1}^k (-1)^j \binom{k}{j} j^{2n-1}}{i(2l+1)}. \quad (25) \]

The convergence radius of (23) is \( \rho_V = \frac{2\pi}{\delta} \), and in the range \( 0 \leq r < \rho_V \) the potential (22) can be approximated with an arbitrary accuracy by a series with a finite number of terms. With the series truncated after the \( r^{2l+1} \) term, the recursion relation (12) takes a form

\[ a_i = -2a_{i-1} + 2(\delta - \lambda)a_{i-2} - 2 \sum_{j=1}^{2l+1} \delta^j g_{j-1} a_{i-(2j+1)}. \quad (26) \]

In Table 3 the numerical results are presented for different values of \( \delta \) at various radii of enclosure \( R < \rho_V \). Numerical stability was achieved by increasing the number of terms both in the series solution (11) and in the potential expansion (23) until the approximate values \( \lambda_{nl} \) for fixed \( R \) become stable to the quoted accuracy. The table also contains the exact eigenvalues \( E_{nl} \) for the unconfined Hulthén potential, obtained analytically \( (l = 0) \) and by numerical integration \( (l \neq 0) \) \[15\].

| \( l \) | \( n = n_r \) | \( \delta \) | \( \lambda_{nl}(4) \) | \( \lambda_{nl}(6) \) | \( \lambda_{nl}(8) \) | \( \lambda_{nl}(12) \) | \( E_{nl} \) |
|-----|-----|-----|-----|-----|-----|-----|-----|
| 0   | 0   | 0.050 | -0.4585448 | -0.4752873 | -0.4753117 | -0.4753125 | -0.4753125 |
|     | 0.075 | -0.4463941 | -0.4631776 | -0.4632024 | -0.4632031 | -0.4632031 |
| 0   | 1   | 0.050 | 0.4447886 | -0.0606327 | -0.0888523 | -0.0975630 | -0.1012500 |
|     | 0.075 | 0.4567303 | -0.0492481 | -0.0776572 | -0.0864942 | -0.0903125 |
| 1   | 0   | 0.050 | 0.1680730 | -0.0802458 | -0.0947675 | -0.0992341 | -0.1010425 |
|     | 0.075 | 0.1800057 | -0.0687394 | -0.0834014 | -0.0879576 | -0.0898478 |

4. Unconfined potentials

Now we come to the discussion of unconfined potentials, namely to the case of a particle with the angular momentum \( l \) in a spherically symmetric potential of the form (11) without any external enclosure. An unconfined system can be also effectively treated by the FM, as demonstrated by the calculation of the ground state energy of the one-dimensional anharmonic oscillator to an enormous precision of 1184-digits \[8\]. Here we show that the method can be implemented in a way that also allows for computing the excited states energies. We take the generalized series (11), as a solution of the radial
Schrödinger equation, which fulfils the boundary condition \( u(\lambda, 0) = 0 \), and consider two ways of imposing the second boundary condition at finite \( r = R \), namely \( u(R, \lambda) = 0 \) or \( u^{(1)}(R, \lambda) = 0 \). At \( R \to \infty \) both conditions are satisfied at the same values of \( \lambda \), which correspond to the energy eigenvalues \( E_{nl} \) of the unconfined system, where \( n = 0, 1, 2, \ldots \).

At finite \( R \) the values of \( \lambda \) are different: let us denote by \( \lambda_{kl} \) the values satisfying
\[
 u(R, \lambda_{kl}) = 0 \quad \text{for} \quad k = 0, 1, \ldots, \tag{27}
\]
and by \( \lambda'_{kl} \) those satisfying
\[
 u^{(1)}(R, \lambda'_{kl}) = 0, \quad \text{for} \quad k = 0, 1, \ldots \tag{28}
\]
In both cases we deal with the Sturm-Liouville eigenvalue problem; the nodes of the function \( u(r, \lambda_{kl}) \) in the radial variable divide thus the domain \((0, R)\) precisely into \( k \)-parts \([10]\), and the same is true for the function \( u(r, \lambda'_{kl}) \). The energy eigenvalues satisfy thus the following inequalities:
\[
 \lambda'_{0l} < \lambda_{0l} < \lambda'_{1l} < \lambda_{1l} < \lambda'_{2l} < \lambda_{2l} < \ldots < \lambda'_{kl} < \lambda_{kl} < \ldots \tag{29}
\]
It is easy to check that the sign of \( u(R, \lambda) \) is opposite to that of \( u^{(1)}(R, \lambda) \), for any value \( \lambda \) lying within \((\lambda'_{kl}, \lambda_{kl})\), which will be called the bounding interval in the following. Whereas, for values of \( \lambda \) in the interval \((\lambda_{kl}, \lambda'_{k+1l})\) the signs of \( u(R, \lambda) \) and \( u^{(1)}(R, \lambda) \) are the same. These properties are best illustrated on Fig.3 in the example of \( u(r, \lambda) \) calculated for the spherical harmonic oscillator with angular momentum \( l = 0 \).

![Figure 3](image_url)

**Figure 3.** Behavior of \( u(R, \lambda) \) (solid line) and \( u^{(1)}(R, \lambda) \) (dashed line) for the spherically symmetric harmonic oscillator with \( \omega = 1 \) and \( l = 0 \) at \( R = 2.5 \). The three first bounding intervals are marked by thick line.

Bound states in the radial potential \( V(r) \) are possible only for \( \lambda < \lim_{r \to \infty} V(r) \). In this case, there exists a point \( R_c \) such that for \( r > R_c \) we have \( V_{eff}(r, l) - \lambda > 0 \) and the sign of \( u^{(2)}(r, \lambda) \) is the same as that of \( u(r, \lambda) \), which implies that for \( r > R_c \) the function \( u(r, \lambda) \) must neither have a local maximum if \( u(R_c, \lambda) > 0 \), nor a local
minimum if \( u(R_c, \lambda) < 0 \). If both \( u(R_c, \lambda) \) and \( u^{(1)}(R_c, \lambda) \) are positive (negative), then \( u(r, \lambda) \) and \( u^{(1)}(r, \lambda) \) tend monotonically to the plus (minus) infinity. Therefore, if the point of imposing the boundary condition, \( R \) is larger than \( R_c \), the following inequality is satisfied
\[
\lambda_{0l}' < E_{0l} < \ldots < \lambda_{kl}' < E_{kl} < \ldots < \lambda_{nl}' < E_{nl} < \lambda_{nl},
\]
where \( \lambda_{nl} < V_{eff}(R, l) \). For increasing \( R \), the energy \( \lambda_{kl}'(R) \) grows and \( \lambda_{kl}(R) \) decreases, approaching the exact eigenvalue \( E_{kl} \) from both sides monotonically. This allows for bounding the energy eigenvalues of an unconfined system with a required precision. With the approximate \( u(R, \lambda) \), obtained by truncating the number of terms in the generalized power series to \( K \), both (27) and (28) are polynomial equations in \( \lambda \). The large set of energy levels can be thus determined numerically by finding the roots of polynomials. Generally, the bounding intervals are larger for higher states but for increasing \( R \) all the bounding interval shrink. We determine thus the new bounding intervals with the value of \( R \) increased by a suitably chosen \( \Delta R \). The iteration procedure is repeated for \( R_i = R + i\Delta R \), until the bounding energies for a chosen state \((k, l)\) become equal to the accuracy desired, which determines its energy with that accuracy. If the procedure does not converge for the state of interest, the number of terms \( K \), which are included in the power series (11) should be increased.

4.1. The Kratzer potential

For demonstrating the convergence of the algorithm previously formulated, we first consider the Schrödinger problem in the Kratzer potential
\[
V(r) = \frac{d_2}{r^2} + \frac{d_1}{r},
\]
for which the exact energy levels are given by
\[
E_{nl} = -2d_2^2(2n + 1 + \sqrt{(2l + 1)^2 + 8d_2})^{-2}, (n = 0, 1, 2, \ldots)
\]
Choosing \( d_1 = -8 \), and \( d_2 = 4 \) as the parameters of the potential (31), we carry out the calculation for the state \((1, 1)\), taking the number of terms in the power series \( K \) suitably large \((K = 160)\) in order to assure the numerical stability. The Table shows with 14-digit precision the values of \( \lambda_{11}(R_i) \), obtained from the condition (27), and those of \( \lambda_{11}'(R_i) \), obtained from (28), for \( R_i = R + i\Delta R \). The bounding interval shrinks very fast and the exact value of energy is easily determined with 14-digit precision, \( E_{11} = -1.4476568219254 \). Figure shows how the deviations from the exact energy monotonically diminish for increasing \( R \), the energy difference \( \lambda_{11}(R) - E_{11} \) approaches zero from above, and \( \lambda_{11}'(R) - E_{11} \) from below.
4.2. Anharmonic oscillator

The unconfined quantum anharmonic oscillator is one of the most frequently discussed quantum systems. Especially the one-dimensional example, being the simplest tractable model of quantum field theory [16], is routinely used for examining the validity of various approximation methods [17], as its exact solution can be numerically determined to an arbitrary accuracy [18,19,20]. The \( D \)-dimensional case is much less studied, generally a spherically symmetric anharmonic potential [10] for different values of the

\[
\lambda_{11}(R) - E_{11}, \quad \lambda'_{11}(R) - E_{11}\text{ to zero, demonstrated in Figure 4.}
\]

| \( R \) | \( \Delta R \) | \( \lambda_{11}(R) - E_{11} \) | \( \lambda'_{11}(R) - E_{11} \) |
|-----|-----|-----------------|-----------------|
| 0   | 0.5 | -1.317826137388 | -1.8092879070838 |
| 1   | 0.5 | -1.3839260262988 | -1.6834926644347 |
| 2   | 0.5 | -1.45178239942994 | -1.5810678698537 |
| 3   | 0.5 | -1.4476568219254  | -1.4476568219254  |
| 4.2 | -0.5 | -1.4476568219254  | -1.4476568219254  |

\( E_{11} = -1.4476568219254 \) for different values of \( R \) and \( \Delta R \).
anharmonicity power $J$ is discussed. The quartic potential ($J = 2$) was studied by means of various approximation methods, e.g. the self-similar approximation [21], the random phase approximation [22], and the artificial perturbation method [23]. There are also a few reports in the literature of the numerically exact results for the quartic [18, 24, 25], sextic ($J = 3$) [1, 24], and octic ($J = 4$) potential [24] in the limited range of the anharmonicity parameter $z$.

Here we show that the FM enables us to determine effectively the spectrum of the unconfined spherical anharmonic oscillator [15] in the wide range of the parameter $z$. With the solution of the Schrödinger equation $u(r, \lambda)$ in the form of the generalized series [19] we determine the numerical values of bound-state energies, using the procedure formulated in the beginning of this section. After checking that the results available in the literature [1, 24, 25] are easily recovered to the quoted accuracy, we performed an extensive calculation of the spectrum of spherically symmetric anharmonic oscillators. The highly accurate results presented here may serve for testing the quality of various approximation methods. Especially challenging test is provided by the data obtained for negative values of the parameter $z$, when the anharmonic potential has a Mexican hat shape. This range was not explored before, and the numerical data for bound-state energies were lacking. Therefore, in table 5 we present our results for several lowest states $(n, l)$ energies of the quartic oscillator ($J = 2$) at negative values of $z$. In table 6 we compare the bound-state energies for oscillators with different anharmonicity powers ($J = 2, 3, 4$) at various values of $z$. The results up to 8-decimal precision are quoted, but it is not difficult to improve the accuracy at will. However, one has to note that the effort of the calculation increases for higher states. The appropriate shrinking of the intervals bounding the higher states energies is achieved only at large $R$, which requires the larger number of terms $K$ to be included in the power series. The computational effort increases strongly, when the parameter $z$ becomes more negative, i.e. for increasing radius of the hat. For example, equality of the values $\lambda_{00}(R)$ and $\lambda_{00}^{\prime}(R)$ with 8-digit accuracy was achieved for $z = -2$ at the radius $R = 3$, which requires $K = 65$, while for $z = -10$ the same is obtained only at $R = 3.9$, which requires $K = 140$.

Table 5. The lowest bound state energies of the quartic oscillator for negative values of $z$.

| $z$ | $E_{00}$  | $E_{01}$  | $E_{02}$  | $E_{03}$  | $E_{04}$  |
|-----|-----------|-----------|-----------|-----------|-----------|
| -10 | -21.88965823 | -21.66759959 | -21.22775192 | -20.57776933 | -19.72742347 |
| -9  | -17.30811508 | -17.05634313 | -16.56006280 | -15.83155272 | -14.88543607 |
| -8  | -13.23757818 | -12.94630409 | -12.37723745 | -11.55086571 | -10.48917435 |
| -7  | -9.68064055  | -9.33403278  | -8.66866023  | -7.71939851  | -6.51858369  |
| -6  | -6.64062824  | -6.21133359  | -5.41635974  | -4.31340468  | -2.94717508  |
Table 6. The low-lying eigenvalues of anharmonic oscillators for certain powers of anharmonicity $2J$ at different values of the parameter $z$

| $J$ | $z$ | $E_{00}$ | $E_{01}$ | $E_{02}$ | $E_{10}$ | $E_{03}$ |
|-----|-----|---------|---------|---------|---------|---------|
| 2   | -5  | -4.11911133 | -3.55958100 | -2.59137576 | -0.21067602 | -1.30027463 |
|     | -4  | -2.10349462 | -1.34175838 | -0.15162331 | 1.57335020 | 1.36098787 |
|     | -3  | -0.54212526 | 0.50094741 | 1.95580851 | 3.17712998 | 3.71671698 |
|     | -2  | 0.66142890 | 2.04064501 | 3.78779723 | 4.66539082 | 5.81395433 |
| 0.1 |     | 2.46463653 | 4.58321826 | 6.96529241 | 7.45891176 | 9.56314673 |
| 0.5 |     | 2.73789227 | 4.99143053 | 7.49177505 | 7.94240398 | 10.19704822 |
|     | 1   | 3.05794573 | 5.47591999 | 8.12171427 | 8.52673739 | 10.95972825 |
| 2   |     | 3.63948205 | 6.37163094 | 9.29940583 | 9.63362791 | 12.39687279 |
| 5   |     | 5.06966367 | 8.63688366 | 12.33685580 | 12.55011513 | 16.15843962 |
| 8   |     | 6.21722563 | 10.49477725 | 14.8706491 | 15.02454165 | 19.33921639 |
| 3   | -8  | -5.00982691 | -4.08581639 | -2.49927339 | 1.27019537 | -0.37612149 |
|     | -5  | -1.39861613 | -0.06070241 | 1.93123653 | 4.23192390 | 4.43629185 |
|     | -2  | 1.24144988 | 3.20845649 | 5.72356878 | 7.05803262 | 8.68689446 |
|     | -1  | 1.94504486 | 4.15238570 | 6.86055253 | 7.97745578 | 9.98954703 |
| 0.1 |     | 2.63985266 | 5.11853012 | 8.04543812 | 8.96977843 | 11.36185573 |
| 1   |     | 3.15630057 | 5.85836853 | 8.96728095 | 9.76393591 | 12.44002444 |
| 4   | -8  | -3.20712029 | -1.83434272 | 0.36915524 | 4.03170882 | 3.24522274 |
|     | -5  | -0.57239228 | 1.19930711 | 3.74932588 | 6.24632114 | 6.93207343 |
|     | -2  | 1.55575737 | 3.85587069 | 6.82325601 | 8.47500053 | 10.35857448 |
|     | -1  | 2.16525909 | 4.66276445 | 7.78250949 | 9.21918447 | 11.4445127 |
| 0.1 |     | 2.78594828 | 5.50821786 | 8.80159788 | 10.03495445 | 12.6073664 |
| 1   |     | 3.25887003 | 6.16887293 | 9.60819432 | 10.69825337 | 13.53482309 |
| 5   | 0.1 | 2.91188167 | 5.81747881 | 9.38031919 | 10.83477815 | 13.54422429 |
|     | 1   | 3.35601445 | 6.42909865 | 10.11830492 | 11.42342067 | 14.38432780 |

Our results for the quartic oscillator are presented graphically in Fig. 5. The excitation energies with respect to the ground state, $E_{nl} - E_{00}$, are plotted in function of the parameter $z$, which covers the range $-15 < z < 25$. The values of $z < 0$ correspond to the Mexican hat, and those of $z > 0$ to the single-well shape of the anharmonic potential (17). It is interesting to note that, in spite of this difference, the dependence of excitation energies on $z$ is smooth at the point separating the two cases, $z = 0$, which corresponds to the strong coupling limit, $g \to \infty$. Instead, the behavior of excitation energies in the weak coupling limit ($|z| \to \infty$) is very different for positive and negative $z$. For $z \to \infty$ we recover the radial harmonic oscillator of the frequency $2z$, which energy
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Figure 5. The behavior $E_{nl} - E_{00}$ in function of $z$, the asymptotic behavior of $E_n - E_0 = n\sqrt{-4z}$ is shown by dashed lines. Two points of level crossing are marked by circles.

eigenvalues are given by

$$E_{nl} \rightarrow (2n + l + \frac{3}{2})\sqrt{2z}, \quad z \rightarrow \infty$$

In Fig. one can observe how the levels with the same $2n + l$ become degenerate for increasing $z$. For $z < 0$ the Mexican hat shaped anharmonic potential has a minimum at $r_{min} = \sqrt{-\frac{z}{2}}$. If $z^3 >> l^2$, the minimum of $V_{eff}$ is close to $r_{min}$ and the effective potential is approximated well by

$$V_{eff}(r) \approx -\frac{z^2}{4} + \frac{1}{2}(-4z)(r - \sqrt{-\frac{z}{2}})^2,$$

which does not depend on $l$, and corresponds to the one-dimensional harmonic oscillator of the frequency $\sqrt{-4z}$. Therefore, in the limit $z \rightarrow -\infty$ we have

$$E_n \rightarrow -\frac{z^2}{4} + (n + \frac{1}{2})\sqrt{-4z}(n = 0, 1, 2, \ldots)$$

In Fig. the grouping of states with different quantum numbers $l$ but the same value of $n$ can be observed for strongly negative values of $z$. For $z \rightarrow -\infty$ all the states in the group approach the asymptotic behavior of $E_n - E_0 = n\sqrt{-4z}$.

One can also notice an interesting phenomenon of level crossing that appears in the range of $z < 0$: at certain negative value of $z$ two adjacent eigenvalues become degenerate. The two examples in Fig. are marked by circles: the crossing point for the states $(1, 0), (0, 3)$, which appears at $z_1 \approx -3.73656382$, and the crossing point for $(1, 0), (0, 4)$, which appears at $z_2 \approx -5.42007803$. The configuration of five lowest states, which for $z > z_1$ is given by $(0, 0), (0, 1), (0, 2), (1, 0), (0, 3)$, changes into
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(0, 0), (0, 1), (0, 2), (0, 3), (1, 0) for \( z_2 < z < z_1 \), and into (0, 0), (0, 1), (0, 2), (0, 3), (0, 4) for \( z < z_2 \). It should be stressed that in the case of one-dimensional anharmonic oscillator the phenomenon of level crossing does not appear, this becomes possible only for systems of \( D \geq 2 \) dimensions.

5. Conclusion

We have shown that the application of the Fröbenius method to the spherically symmetrical potentials of the form \( V(r) = \frac{d_{-2}}{r^2} + \frac{d_{-1}}{r} + \sum_{i=0}^{\infty} d_i r^i \) allows an easy determination of the energy spectrum. This was demonstrated first for systems enclosed in a spherical box of the radius \( R \), by studying the confined harmonic and anharmonic oscillators and Hulthén potential. With the increasing radius of confinement the bound states energies have been shown to approach those of the corresponding unconfined systems. Even in the case of the Hulthén potential, when the convergence radius of the potential is finite, we obtain quite good approximations to the low-lying spectrum of the unconfined potential, if the screening is not too strong. Later, we developed an efficient scheme for computing eigenvalues of the Schrödinger equation for unconfined potentials with a controlled accuracy. The method allowed us to determine the low-lying states energies of spherically symmetric anharmonic oscillators with very high accuracy and moderate effort. Determination of energies becomes computationally more demanding for higher states, since more terms have to be included in the generalized power series. Our calculations cover a broad range of anharmonic parameters, both in the case of single well potential and for the Mexican hat shape. In the later case the computational effort increases strongly with the increasing radius of the hat.

The method presented in this work can be easily applied for computing the precise spectrum of other spherically symmetric potentials. In the present work, we have studied the case of three-dimensional space but the calculation of energy levels in the two-dimensional case can be performed along similar lines. The results in even and odd higher dimension \( D \) can be easily derived from those in 2– and 3–dimensional space, respectively, via the transformation \( l \to l + \frac{D-3}{2} \). One has to add that the method can be also used to determine the approximate wave functions. After substituting the calculated bound-state energy to the recursion relation (12) the coefficients of the generalized wave functions \( (11) \) can be successively determined in order to obtain the unnormalized wave function as a sum of the series.

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