On the calculation of bound-state energies supported by hyperbolic double well potentials

Francisco M. Fernández∗
INIFTA, DQT, Sucursal 4, C.C 16,
1900 La Plata, Argentina

Abstract

We obtain eigenvalues and eigenfunctions of the Schrödinger equation with a hyperbolic double-well potential. We consider exact polynomial solutions for some particular values of the potential-strength parameter and also numerical energies for arbitrary values of this model parameter. We test the numerical method by means of a suitable exact asymptotic expression for the eigenvalues and also calculate critical values of the strength parameter that are related to the number of bound states supported by the potential.

1 Introduction

In the last years there has been interest in quantum-mechanical models with hyperbolic potentials [1–7]. The reason is that some of them appear to be useful in some physical applications [1, 2]. Under suitable transformations the resulting eigenvalue equations are exactly or conditionally solvable [1–7]. The Schrödinger equation can be transformed into a Kummer’s differential equation [2] or a confluent Heun equation [1, 3–7] and the Frobenius method (power-series approach) leads to a three-term recurrence relation for the expansion

∗fernande@quimica.unlp.edu.ar
coefficients \[3,5–7\]. This fact enables one to obtain exact polynomial solutions by a suitable truncation condition. Besides, it is also possible to obtain numerical solutions for all the states of the problem from the same tree-term recurrence relation through an alternative truncation condition \[7\].

The purpose of this paper is to investigate the relationship between the energies associated with the exact polynomial solutions and those obtained numerically from the same three-term recurrence relation. In particular, we are interested in the accuracy and usefulness of the numerical method. In section \[2\] we briefly discuss the model and the transformation of the Schrödinger equation into a convenient eigenvalue equation that is suitable for the application of the Frobenius method. From a suitable truncation condition we obtain exact polynomial solutions for some particular bound states \[3,5–7\]. In section \[3\] we test a numerical method for the calculation of all the bound-state eigenvalues from the three-term recurrence relation for the coefficients of the Frobenius expansion \[7\]. Finally, in section \[4\] we summarize the main results and draw conclusions.

## 2 The model

Following Downing \[3\] we consider the one-dimensional Schrödinger equation

\[
- \frac{\hbar^2}{2m} \psi''(x) + V(x)\psi(x) = E\psi(x), \quad V(x) = -V_0 \frac{\sinh^4 (x/d)}{\cosh^6 (x/d)},
\]

for a particle of mass \(m\) in a hyperbolic potential with two model parameters \(V_0 > 0\) and \(d > 0\) that determine its depth and width, respectively. This potential exhibits a barrier at \(x = 0\), \(V(0) = 0\), between two minima at \(x_\pm = d \ln (\sqrt{3} \pm \sqrt{2})\) of depth \(V(x_\pm) = -4V_0/27\). Since \(V(x \rightarrow \pm \infty) = 0\) then there will be bound-state energies in the interval \(-4V_0/27 < E < 0\).

If we define the dimensionless coordinate \(z = x/d\), the dimensionless parameter \(v_0 = 2md^2V_0/\hbar^2\) and the dimensionless energy \(\epsilon = 2md^2E/\hbar^2\) the resulting dimensionless equation \[8\]

\[
- \varphi''(z) + v(z)\varphi(z) = \epsilon\varphi(z), \quad v(z) = -v_0 \frac{\sinh^4 (z)}{\cosh^6 (z)},
\]

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clearly shows that there is just one relevant parameter, \( v_0 \), and not two as some authors appeared to suggest \[3,5,7\]. In fact, the problem reduces to calculating \( \epsilon (v_0) \) and the width parameter is only necessary in order to obtain \( E(V_0, d) = \hbar^2 \epsilon (v_0) / (2md^2) \) \[6,8\]. It is clear that the dimensionless bound-state energies will appear in the interval \(-4v_0/27 < \epsilon < 0\).

According to the Hellmann-Feynman theorem \[9,10\] the eigenvalues decrease with the potential-strength parameter as

\[
\frac{d\epsilon}{dv_0} = \frac{\sinh^4(z)}{\cosh^2(z)}.
\]

(3)

By means of the change of variables \( \xi = 1/\cosh(z) \) the dimensionless equation (2) becomes

\[
4\xi^2 (1 - \xi) u''(\xi) + 2\xi (2 - 3\xi) u'(\xi) + \left[ \epsilon + v_0 (\xi - 1)^2 \right] u(\xi) = 0,
\]

(4)

where \( 0 < \xi \leq 1 \). From a further transformation \[3\]

\[
u(\xi) = \xi^{\beta/2} \exp \left( \frac{\alpha}{2} \xi \right) y(\xi),
\]

(5)

where \( \beta = \sqrt{-\epsilon} \) and \( \alpha^2 = v_0 \), we obtain the more convenient equation

\[
4\xi^2 (1 - \xi) y''(\xi) - 2\xi \left[ 2\alpha \xi (\xi - 1) + 2\beta (\xi - 1) + 3\xi - 2 \right] y'(\xi)

- \left[ \alpha^2 (\xi - 1) + \alpha (2\beta (\xi - 1) + 3\xi - 2) + \beta^2 + \beta \right] y(\xi) = 0.
\]

(6)

It follows from the bounds to the dimensionless energies discussed above that

\[
0 < \beta < \frac{2|\alpha|}{\sqrt{27}}.
\]

(7)

The solution \( y(\xi) \) can be expanded in a Taylor series about the origin

\[
y(\xi) = \sum_{j=0}^{\infty} c_j \xi^j,
\]

(8)

and the expansion coefficients \( c_j \) satisfy the three-term recurrence relation

\[
c_{j+2}(\alpha, \beta) = A_j(\alpha, \beta)c_{j+1}(\alpha, \beta) + B_j(\alpha, \beta)c_j(\alpha, \beta),
\]

(9)

\[
j = -1, 0, 1, 2, \ldots, c_{-1} = 0, \quad c_0 = 1,
\]

\[
A_j(\alpha, \beta) = \frac{(\beta + 2j + 3)(2\alpha - \beta - 2(j + 1)) + \alpha^2}{4(\beta + j + 2)(j + 2)},
\]

\[
B_j(\alpha, \beta) = \frac{\alpha(\alpha + 2\beta + 4j + 3)}{4(\beta + j + 2)(j + 2)}.
\]
For those physically acceptable solutions to the truncation conditions \( c_n \neq 0, c_{n+1} = 0 \) and \( c_{n+2} = 0 \), \( n = 0, 1, \ldots \), the series reduces to a polynomial of degree \( n \). It follows from these conditions that \( B_n(\alpha, \beta) = 0 \) which forces a relationship between \( \alpha \) and \( \beta \). We arbitrarily choose

\[
\beta = \beta_n = -\frac{\alpha + 4n + 3}{2},
\]

so that

\[
A_{j,n}(\alpha) = -\frac{\alpha^2 - 8\alpha (3j - 3n + 2) + (4j - 4n + 1)(4j - 4n + 3)}{8(\alpha - 2j + 4n - 1)(j + 2)},
\]

\[
B_{j,n}(\alpha) = \frac{2\alpha (n - j)}{(\alpha - 2j + 4n - 1)(j + 2)}.
\]

The coefficient \( c_{n+1} \) is a rational function of \( \alpha \) and its numerator is a polynomial of degree \( 2(n+1) \); therefore, the remaining condition \( c_{n+1} = 0 \) has \( 2(n+1) \) solutions \( \alpha_{n,i} \), \( i = 1, 2, \ldots, 2(n+1) \). Numerical calculation suggests that all the roots are real; however, not all of them are physically acceptable. It follows from equations (7) and (10) that there are exact polynomial solutions only for those roots that satisfy

\[
-\frac{27 + 12\sqrt{3}}{11} (4n + 3) < \alpha_{n,i} < -(4n + 3).
\]

The polynomial solutions to equation (6) are of the form

\[
y^{(n,i)}(\xi) = \sum_{j=0}^{n} c_j (\alpha_{n,i}) \xi^j,
\]

for those values of \( \alpha_{n,i} \) in the interval given in equation (12). It is worth noticing that present hyperbolic potential supports at least one bound state for any positive value of \( v_0 \) (see, for example, [6] and references therein).

Since \( \xi \) is an even function of \( z \) then all the solutions obtained in the way just described are even functions of \( z \). It is obvious that there should be even \( \varphi^e(z) \) and odd \( \varphi^o(z) \) solutions to the dimensionless eigenvalue equation (2) and the approach just outlined is unable to provide the latter. An alternative strategy is based on the more convenient variable \(-1 < \zeta = \tanh(z) < 1\) that enables us to obtain both even and odd solutions [3]. However, it is possible to obtain
also the odd solutions from the transformation just discussed. In fact, since \( \varphi^0(0) = 0 \) and \( \xi(0) = 1 \) it is only necessary to force a zero at \( \xi = 1 \) as discussed by Wen et al. \[4\] and Hall and Saad \[6\]. This more general approach is outlined in Appendix A.

Figure 1 shows that the highest roots \( \epsilon(n,i) \) (for the exact polynomial solutions) follow a neat decreasing curve in terms of \( \alpha^2_{n,i} \). However, this curve has no physical meaning as shown in what follows.

3 Numerical calculation

The truncation condition discussed in the preceding section only yields some particular energies \( \epsilon(n,i) \) for some particular values of the strength parameter \( v_0^{(n,i)} = \alpha^2_{n,i} \), provided that the values of \( \alpha_{n,i} \) satisfy the bounds in equation \[12\]. Such results are almost useless if one is not able to identify and organize them properly. Kufel et al. \[7\] proposed an approach for the calculation of all the bound-state energies that is similar to a procedure developed some time ago by Myrheim et al. \[11\]. The strategy consists of setting the desired value of \( \alpha \), calculating the coefficients \( c_j \), \( j = 0, 1, \ldots, N \), from the recurrence relation \[9\] and then solving the equation \( c_N = 0 \) for \( \beta \). Those sequences of roots \( \beta^{(N,j)} \), \( N = N_I, N_I + 1, \ldots \) that converge to a limit in the range given by equation \[7\] are expected to yield the energy eigenvalues for the chosen value of \( \alpha \).

Figure 2 shows numerical eigenvalues for two values of \( v_0 \) (blue crosses). This figure also shows the exact eigenvalues stemming from the truncation condition discussed in the preceding section (red circles). Notice that the exact eigenvalues follow well defined curves (the highest one shown in Figure 1 in a smaller scale) which, in principle, do not have any physical meaning because they connect bound states with different quantum numbers.

In order to test the validity of this numerical calculation of the energies supported by the hyperbolic double well we resort to a simple asymptotic expression, valid for sufficiently large values of \( v_0 \). Under such condition we expand
the potential in a Taylor series about either minima

\[ V(z) = v_0 \left[-\frac{4}{27} + \frac{8}{27} (z - z_\pm)^2 + \ldots \right], \quad z_\pm = \ln \left(\sqrt{3} \pm \sqrt{2}\right), \quad (14) \]

and apply the harmonic approximation. In this way we obtain approximate asymptotic eigenvalues

\[ \epsilon_\text{asymp} = -\frac{4}{27} v_0 + 2 \sqrt{\frac{2v_0}{27}} (2\nu + 1), \quad \nu = 0, 1, \ldots, k. \quad (15) \]

Figure 3 shows that the numerical values of \( \epsilon_0 \) (blue squares) already agree with \( \epsilon_0 \text{asymp} \) (green line) which strongly suggests that the truncation condition \( c_N = 0 \) is suitable for obtaining the eigenvalues of the hyperbolic double well (\( N = 10 \) was sufficient for the scale of this figure). This figure also shows some exact results (red circles) given by the truncation condition of the preceding section. As a further test of the method just outlined we have also verified that the energies obtained in this way agree with those coming from the widely tested Riccati-Padé method [12].

According to the Hellmann-Feynman theorem [3] the bound-state energies \( \epsilon_\nu \) decrease with \( v_0 \). For any value of \( v_0 \) there is at least one bound state of even symmetry and the number of bound states supported by the potential increases with \( v_0 \) (see, for example, Hall and Saad [6] and references therein for a discussion of this issue). Consequently, there are critical values of the potential-strength parameter \( v_0 = v_{0,K}, K = 1, 2, \ldots \), such that \( \epsilon_K = 0 \). Their meaning is that there is just one bound state for \( v_0 \leq v_{0,1} \) and \( K + 1 \) bound states for \( v_{0,K} < v_0 < v_{0,K+1} \). The numerical method outlined above enables us to obtain the critical values \( \alpha_K \) of \( \alpha \) in a simple way. We simply set \( \beta = 0 \) and solve \( c_N = 0 \) for \( \alpha \) for sufficiently large values of \( N \). From a straightforward calculation with \( N \leq 36 \) we estimated \( \alpha_2 = -5.272715881, \alpha_4 = -9.398121349, \alpha_6 = -13.455570 \) and \( \alpha_8 = -17.4897 \). On using the three-term recurrence relation with the factors given in equation \( \text{A.3} \) and \( \gamma = 1 \) we obtain \( \alpha_1 = -20.73164811, \alpha_3 = -6.181847266, \alpha_5 = -10.22002699, \alpha_7 = -14.2405704 \) and \( \alpha_9 = -18.25373 \).
4 Conclusions

In this paper we have discussed the exact polynomial solutions to the Schrödinger equation with the hyperbolic double well potential shown in equation (2). In particular, we focused on the bounds to the physically acceptable values \( \alpha_{n,i} \) of the parameter \( \alpha = -\sqrt{v_0} \) and showed that the energies \( \epsilon^{(n,i)} \) appear on some decreasing curves on the \( v_0 - \epsilon \) plane, though their meaning is not clear to us. We also compared these exact eigenvalues with some numerical results \( \epsilon_\nu (v_0) \) provided by a simple method based on the three-term recurrence relation [7]. In order to test the validity of the numerical approach we resorted to an exact asymptotic expression for the eigenvalues, valid for sufficiently deep wells. The numerical approach proves useful for the calculation of the critical values \( v_{0,K} = \alpha_K^2 \) of the strength parameter \( v_0 \) that are related to the number of bound states supported by the potential.

References

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A Even and odd states

In order to obtain odd states from the procedure outlined in section 2 we have to force a zero at $\xi = 1$, which can be easily done by the transformation

$$u(\xi) = \xi^{\beta/2} (1 - \xi)^{\gamma/2} \exp \left( \frac{\alpha^2}{2} \xi \right) y(\xi), \quad (A.1)$$

where $\beta = \sqrt{-\varepsilon}$, $\alpha^2 = v_0$ (as before) and $\gamma(\gamma - 1) = 0$. When $\gamma = 0$ we recover the ansatz of section 2 for even states and $\gamma = 1$ gives us the odd states. The differential equation becomes

$$4\xi^2 (1 - \xi) y''(\xi) - 2\xi [2\alpha \xi (\xi - 1) + 2\beta (\xi - 1) + 2\gamma \xi + 3\xi - 2] y'(\xi)$$

$$- \xi \{ \alpha^2 (\xi - 1) + \alpha [2\beta (\xi - 1) + 2\gamma \xi + 3\xi - 2] + \beta^2 + \beta (2\gamma + 1)$$

$$+ \gamma(\gamma + 1) \} y(\xi). \quad (A.2)$$

On arguing as in section 2 we obtain a similar three-term recurrence relation with

$$A_j(\gamma, \alpha, \beta) = - \frac{\alpha^2 + 2\alpha (\beta + 2j + 3) - \beta^2 - \beta (2\gamma + 4j + 5)}{4(\beta + j + 2)(j + 2)}$$

$$+ \frac{\gamma^2 + \gamma (4j + 5) + 2(\beta + j + 1)(2j + 3)}{4(\beta + j + 2)(j + 2)},$$

$$B_j(\gamma, \alpha, \beta) = \frac{\alpha (\alpha + 2\beta + 2\gamma + 4j + 3)}{4(\beta + j + 2)(j + 2)}. \quad (A.3)$$
Upon choosing
\[ \beta = \beta_n = -\frac{\alpha + 2\gamma + 4n + 3}{2}, \] (A.4)
we have
\[ A_{j,n}(\gamma, \alpha) = -\frac{\alpha^2 + 8\alpha (\gamma - 3j + 3n - 2) + (4j - 4n - 1)(4j - 4n + 3)}{8(\alpha + 2\gamma - 2j + 4n - 1)(j + 2)}, \]
\[ B_{j,n}(\gamma, \alpha) = \frac{2\alpha (n - j)}{(\alpha + 2\gamma - 2j + 4n - 1)(j + 2)}, \] (A.5)
and the tree-term recurrence relation yields exact polynomial solutions for \( y(\xi) \).
Only the roots \( \alpha_{n,i} \) of \( c_{n+1} = 0 \) that satisfy
\[ -\frac{27 + 12\sqrt{3}}{11}(4n + 3 + 2\gamma) < \alpha_{n,i} < -(4n + 3 + 2\gamma), \] (A.6)
are physically acceptable. These bounds apply only to the exact polynomial solutions.

We can also obtain numerical eigenvalues for both even and odd states and any \( v_0 > 0 \) from the roots of \( c_N = 0 \) as indicated in section 3.
Figure 2: Eigenvalues from the truncation method (red points) and numerical ones for $v_0 = 1764$ and $v_0 = 2809$ (blue crosses)

Figure 3: Ground state calculated numerically (blue squares), by means of the exact truncation condition (red points) and from the asymptotic expression (green line)