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Exact solutions of the Schrödinger equation for a class of hyperbolic potential well

Xiao-Hua Wang(王晓华)[1], Chang-Yuan Chen(陈昌远)[1,†], Yuan You(尤源)[1], Fa-Lin Lu(陆法林)[1], Dong-Sheng Sun(孙东升)[1], and Shi-Hai Dong(董世海)[2,3,‡]

[1] *School of Physics and Electronic Engineering, Yancheng Teachers University, Yancheng* 224007, *China*
[2] *Research Center for Quantum Physics, Huzhou University, Huzhou* 313000, *China*
[3] *Laboratorio de Información Cuántica, CIDETEC, Instituto Politécnico Nacional, UPALM, C.P* 07700, *CDMX, Mexico*

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We propose a new scheme to study the exact solutions of a class of hyperbolic potential well. We first apply different forms of function transformation and variable substitution to transform the Schrödinger equation into a confluent Heun differential equation and then construct a Wronskian determinant by finding two linearly dependent solutions for the same eigenstate. And then in terms of the energy spectrum equation which is obtained from the Wronskian determinant, we are able to graphically decide the quantum number with respect to each eigenstate and the total number of bound states for a given potential well. Such a procedure allows us to calculate the eigenvalues for different quantum states via Maple and then substitute them into the wave function to obtain the expected analytical eigenfunction expressed by the confluent Heun function. The linearly dependent relation between two eigenfunctions is also studied.

Keywords: hyperbolic potential well, Schrödinger equation, Wronskian determinant, confluent Heun function

PACS: 03.65.Ge, 03.65.Db, 02.30.–f, 02.60.Jh **DOI:** 10.1088/1674-1056/ac3392

1. Introduction

As we know, one of the fundamental tasks of quantum mechanics is to explore the exact solution of the Schrödinger equation for all kinds of potential fields by using different methods.[1–3] Because the hyperbolic potential well has important applications in physics,[4–8] the symmetric and asymmetric single and double-well shapes have been studied widely by many methods, such as asymptotic iteration method (AIM), Bethe ansatz method, and the confluent Heun function approach that can be broken into an N degree polynomial under certain constraints, *etc*.[9–23] It should be emphasized that these methods focus on how to obtain more accurate eigenvalues but pay less attention to explicit eigenfunctions except for the modified Pöschl–Teller potential.[24–26]

In general, the one-dimensional (1D) Schrödinger equation for a non-relativistic particle of mass M subject to a hyperbolic potential well $U_q(x;u,L)$ is given by

$$-\frac{\hbar^2}{2M}\frac{\mathrm{d}^2\psi(x)}{\mathrm{d}x^2}+U_q(x;u,L)\psi(x)=E\psi(x),\quad \psi(\pm\infty)=0, \tag{1}$$

where

$$U_q(x;u,L) = -\frac{\hbar^2 u}{2ML^2}\frac{1}{\cosh^4(x/L)},-\frac{\hbar^2 u}{2ML^2}\frac{\sinh^2(x/L)}{\cosh^4(x/L)},$$
$$-\frac{\hbar^2 u}{2ML^2}\left[1-\frac{\sinh^4(x/L)}{\cosh^4(x/L)}\right],\quad q=1,2,3. \tag{2}$$

The parameters u and L denote the depth and width of potential well $U_q(x;u,L)$ respectively, and u is a dimensionless parameter. For these potential wells, only in Ref. [13] AIM was used to study the eigenvalue of potential well U_2, and the other two have never been reported to our best knowledge. Taking a simple change of variable $x'=x/L$ transforms equation (1) into a single parameter Schrödinger equation

$$-\frac{\mathrm{d}^2\psi(x')}{\mathrm{d}x'^2}+U(x';u)\psi(x')=\varepsilon\psi(x'),\quad \psi(\pm\infty)=0, \tag{3}$$

where

$$U_q(x';u)=-\frac{u}{\cosh^4(x')},-\frac{u\sinh^2(x')}{\cosh^4(x')},-u\left[1-\frac{\sinh^4(x')}{\cosh^4(x')}\right],$$
$$\varepsilon=2ML^2E/\hbar^2<0. \tag{4}$$

We notice that $U_q(x';u)$ is an even function without singularity as illustrated in Fig. 1. On the other hand, it is found that the $U_{1,3}$ are both single well with potential depth u, and U_2 is a double well with potential depth $u/4$. Referring to Refs. [1–3,27,28], the number of bound states is finite for the potential well U_q. No matter how shallow the potential well is, there exists at least one even parity bound state. According to the basic principles of quantum mechanics, the bound state is non-degenerate and the eigenfunction satisfies $\psi_n(-x')=(-1)^n\psi_n(x')$, where n is the number of the nodes of the wave function.

This paper is organized as follows: In Section 2 based on our recent works,[29–33] taking U_1 as a typical example, we describe how to accurately solve the bound states of the

†Corresponding author. E-mail: chency@yctu.edu.cn
‡Corresponding author. E-mail: dongsh2@yahoo.com

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Schrödinger equation. For this purpose, the first step is to transform the corresponding Schrödinger equation into a confluent Heun differential equation by using different forms of variable substitution and function transformation and then obtain two linearly dependent solutions for the same eigenstate. The second step is to construct a Wronskian determinant from those two linearly dependent solutions and then based on it to obtain an energy spectrum equation. As a result, the quantum number corresponding to each eigenstate and the total number of bound states can be illustrated graphically through studying this energy equation. The third step is to calculate the exact energy ε of each eigenstate with the aid of Maple. Finally, by substituting the obtained energy ε into the wave function we are able to get the explicit wave function expressed by the confluent Heun function and also study their linear correlation. In Sections 3 and 4, the exact solutions of potential wells U_2 and U_3 are investigated briefly in a similar way. The conclusions of this paper are finally given in Section 5.

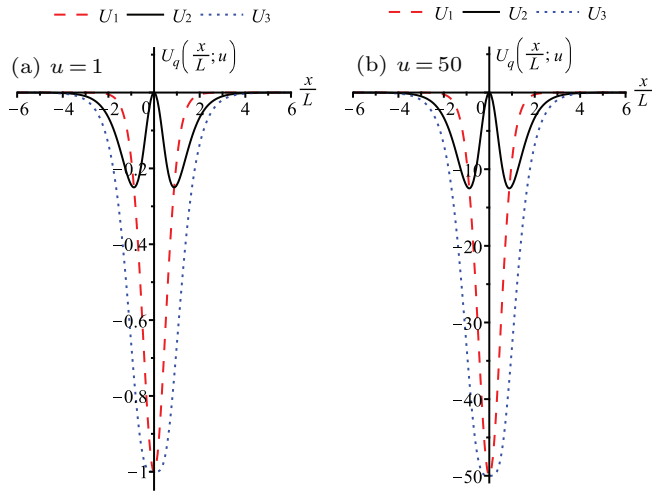


Fig. 1. The plot of the hyperbolic potential wells with two different depth u.

2. Exact solutions of potential well U_1

Substituting U_1 into Eq. (3) allows us to obtain the following equation:

$$\frac{\mathrm{d}^2\psi(x')}{\mathrm{d}x^2}+\frac{u}{\cosh^4(x')}\psi(x')-m^2\psi(x')=0, \tag{5}$$

where

$$m=\sqrt{-\varepsilon}>0, \quad \varepsilon=2ML^2E/\hbar^2<0. \tag{6}$$

Taking a new variable $y=\tanh(x')\in[-1,1]$ for $x'\in(-\infty,\infty)$ allows us to obtain the following equation:

$$(1-y^2)\frac{\mathrm{d}^2\psi(y)}{\mathrm{d}y^2}-2y\frac{\mathrm{d}\psi(y)}{\mathrm{d}y} +\left[u-uy^2-\frac{m^2}{1-y^2}\right]\psi(y)=0. \tag{7}$$

Considering the boundary conditions $\psi|_{x'\to\pm\infty}=\psi|_{y=\pm1}=0$, we first take the wave function of the form $\psi(y)=(1-y^2)^{m/2}\mathrm{e}^{\mathrm{i}\sqrt{u}y}F(y)$ and then substitute this into Eq. (7). This enables us to obtain the following differential equation for $F(y)$:

$$(1-y^2)F''(y)+[\mathrm{i}2\sqrt{u}(1-y^2)-2(m+1)y]F'(y) +[-\mathrm{i}2\sqrt{u}(m+1)y-m(m+1)]F(y)=0. \tag{8}$$

By taking $z=(1-y)/2\in[1,0]$, $y\in[-1,1]$, equation (8) can be further modified as

$$F''(z)+\left(-\mathrm{i}4\sqrt{u}+\frac{m+1}{z}+\frac{m+1}{z-1}\right)F'(z) +\left(\frac{-\mathrm{i}2\sqrt{u}(m+1)-m(m+1)}{z} +\frac{-\mathrm{i}2\sqrt{u}(m+1)+m(m+1)}{z-1}\right)F(z)=0. \tag{9}$$

Compared this with the confluent Heun differential equation[15,16,34–36]

$$\frac{\mathrm{d}^2H(z)}{\mathrm{d}z^2}+\left[\alpha+\frac{\beta+1}{z}+\frac{\gamma+1}{z-1}\right] \times\frac{\mathrm{d}H(z)}{\mathrm{d}z}+\left[\frac{\mu}{z}+\frac{\nu}{z-1}\right]H(z)=0, \tag{10}$$

we are able to find the corresponding parameters as follows:

$$\begin{aligned}&\alpha=-\mathrm{i}4\sqrt{u}, \quad \beta=m, \quad \gamma=m,\\ &\mu=-\mathrm{i}2\sqrt{u}(m+1)-m(m+1),\\ &\nu=-\mathrm{i}2\sqrt{u}(m+1)+m(m+1).\end{aligned} \tag{11}$$

Since $\beta=m\geq0$, the solutions of Eq. (9) are given by

$$\begin{aligned}F(z)&=\mathrm{HeunC}(\alpha,\beta,\gamma,\delta,\eta,z)\\ &=\sum_{n=0}^{\infty}\upsilon_n(\alpha,\beta,\gamma,\delta,\eta)z^n, \quad 0\leq z<1,\end{aligned} \tag{12}$$

where

$$\begin{aligned}&\delta=\mu+\nu-[\alpha(\beta+\gamma+2)/2]=0,\\ &\eta=[\alpha(\beta+1)/2]-[(\beta+\gamma+\beta\gamma)/2]-\mu=m^2/2.\end{aligned} \tag{13}$$

In particular, $\mathrm{HeunC}(\alpha,\beta,\gamma,\delta,\eta,0)=1$. The coefficients υ_n satisfy a three-term recurrence relation $A_n\upsilon_n=B_n\upsilon_{n-1}+C_n\upsilon_{n-2}$ with initial coefficients $\upsilon_{-1}=0,\upsilon_0=1$. Thus, we can only obtain the convergent solutions of Eq. (7) at $z=0$ $(y=1,x\to\infty)$

$$\psi_1(y)=(1-y^2)^{m/2}\mathrm{e}^{\mathrm{i}\sqrt{u}y}F(1), \tag{14}$$

where

$$F(1)=\mathrm{HeunC}\left(-\mathrm{i}4\sqrt{u},m,m,0,m^2/2,(1-y)/2\right). \tag{15}$$

Let us study Eq. (8) in another way, *i.e.*, taking another new variable $z'=1-z=(1+y)/2\in[0,1]$ in Eq. (8) will make it rearranged as

$$\frac{\mathrm{d}^2F(z')}{\mathrm{d}z'^2}+\left[\alpha'+\frac{\beta'+1}{z'}+\frac{\gamma'+1}{z'-1}\right]\frac{\mathrm{d}F(z')}{\mathrm{d}z'}$$

$$+\left[\frac{\mu'}{z'}+\frac{\eta'}{z'-1}\right]F(z')=0, \tag{16}$$

where

$$\begin{aligned}
&\alpha'=-\alpha=\mathrm{i}4\sqrt{u},\quad \beta'=\gamma=m,\quad \gamma'=\beta=m,\\
&\mu'=-\nu=\mathrm{i}2\sqrt{u}(m+1)-m(m+1),\\
&\nu'=-\mu=\mathrm{i}2\sqrt{u}(m+1)+m(m+1),\\
&\delta'=-\delta=0,\quad \eta'=\eta+\delta=m^2/2.
\end{aligned} \tag{17}$$

Likewise, because of $\beta'=m\geq 0$ the solutions of Eq. (16) are also given by the confluent Heun functions

$$\begin{aligned}
F(z') &= \mathrm{HeunC}(\alpha',\beta',\gamma',\delta',\eta',z')\\
&= \mathrm{HeunC}(-\alpha,\gamma,\beta,-\delta,\eta+\delta,1-z),\\
&\quad 0\leq z'<1.
\end{aligned} \tag{18}$$

Thus, the convergent solutions of Eq. (7) at $z'=0$ ($z=1, y=-1, x\to-\infty$) are given by

$$\psi_2(y)=(1-x^2)^{m/2}\,\mathrm{e}^{\mathrm{i}\sqrt{u}y}F(2), \tag{19}$$

where

$$F(2)=\mathrm{HeunC}(\mathrm{i}4\sqrt{u},m,m,0,m^2/2,(1+y)/2). \tag{20}$$

We notice that both equations (14) and (19) are solutions to the differential equation (7). This is a typical Sturm–Liouville problem, *i.e.*, the eigenvalues are the real numbers; the eigenstates are not degenerate and the eigenfunctions will form an orthonormalized complete set. Thus, these two eigenfunctions belonging to the same eigenstate except for having different mathematical expressions should be convergent for the same eigenvalue ε at $y=\pm1(x'\to\pm\infty)$ and must also be linearly dependent within the interval $y\in(-1,1)$.[37–39] For two nonzero constants C_1 and C_2, the solutions of Eq. (7) has the relation $C_1\psi_1(x')+C_2\psi_2(x')=0$. Substitution of Eqs. (14) and (19) into it leads to $C_1F(1)+C_2F(2)=0$, whose first derivative $C_1F'(1)+C_2F'(2)=0$. From these two relations we obtain a useful Wronskian determinant

$$\begin{vmatrix} F(1) & F(2)\\ F'(1) & F'(2)\end{vmatrix}=0, \tag{21}$$

from which we have

$$\begin{aligned}
&\mathrm{HeunC}(-\mathrm{i}4\sqrt{u},m,m,0,m^2/2,(1-y)/2)\\
&\times\mathrm{HeunCPrime}(\mathrm{i}4\sqrt{u},m,m,0,m^2/2,(1+y)/2)\\
&+\mathrm{HeunC}(\mathrm{i}4\sqrt{u},m,m,0,m^2/2,(1+y)/2)\\
&\times\mathrm{HeunCPrime}(-\mathrm{i}4\sqrt{u},m,m,0,m^2/2,(1-y)/2)=0,
\end{aligned} \tag{22}$$

where we have considered the differentiation rules for the composite function and the relevant definitions in Maple. For convenience, we take $y=0$ in Eq. (22) to calculate the eigenvalues since they are linearly dependent inside the interval $y\in(-1,1)$. For a given value u, the following ε-dependent function can be used to determine the energy ε

$$\begin{aligned}
f(\varepsilon) &= \mathrm{HeunC}(-\mathrm{i}4\sqrt{u},m,m,0,m^2/2,1/2)\\
&\quad\times\mathrm{HeunCPrime}(\mathrm{i}4\sqrt{u},m,m,0,m^2/2,1/2)\\
&\quad+\mathrm{HeunC}(\mathrm{i}4\sqrt{u},m,m,0,m^2/2,1/2)\\
&\quad\times\mathrm{HeunCPrime}(-\mathrm{i}4\sqrt{u},m,m,0,m^2/2,1/2).
\end{aligned} \tag{23}$$

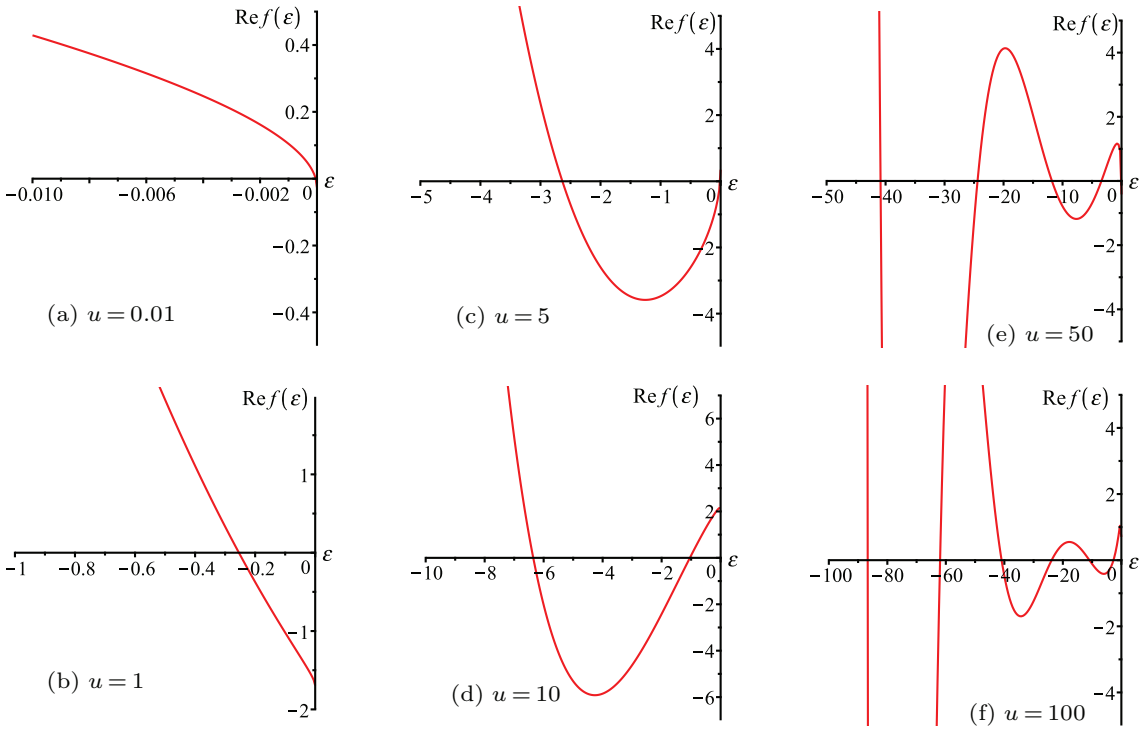


Fig. 2. Plot of Re $f(\varepsilon)$ as a function of ε with different depths u for the potential well U_1.

Table 1. Precise values of the dimensionless energy ε for the potential well U_1.

n	$u=0.01$	$u=1$	$u=5$	$u=10$	$u=50$	$u=100$
	–0.0000 4407	–0.2540 2624	–2.6351 4950	–6.3525 6769	–40.8554 9890	–86.7195 7198
1			–0.0075 8876	–1.0420 5500	–24.4103 0217	–61.9730 7338
2					–11.7980 4314	–40.9416 4410
3					–3.4081 3296	–23.8295 0133
4					–0.0109 5309	–10.9276 9728
5						–2.6966 5748

For $-u<\varepsilon<0$, the intersection of the function $\mathrm{Re}\,f(\varepsilon)$ with the 'ε axis' is nothing but the definite eigenvalue. For a given u, the number of intersection to 'ε axis' is finite, which corresponds to the number of bound states (see Fig. 2). For example, only one bound state exists for $u=0.01$ and 1, two bound states for $u=5$ and 10, while six bound states for $u=100$, *etc*. As a convention, the leftmost intersection is the ground state with the lowest energy (*i.e.* $n=0$), the next followed intersection is the first excited state with the quantum number $n=1$. From Eq. (22), the precise values of corresponding quantum number n and energy ε for different depth u can be calculated by using Maple, the results are listed in Table 1.

Before ending this part, let us study the linear dependence between these two eigenfunctions as displayed in Fig. 3. Since both equations (14) and (19) are complex functions, after the calculated eigenvalues are substituted into them, we find that their real and imaginary parts have the following relations:

$$\begin{aligned}\mathrm{Re}\left[\psi_1(x/L)\right]&=(-1)^n\,\mathrm{Re}\left[\psi_2(x/L)\right],\\ \mathrm{Im}\left[\psi_1(x/L)\right]&=(-1)^{n+1}\,\mathrm{Im}\left[\psi_2(x/L)\right].\end{aligned}\tag{24}$$

As what follows, we are ready to study other two potential wells $U_{2,3}$ as the case of U_1.

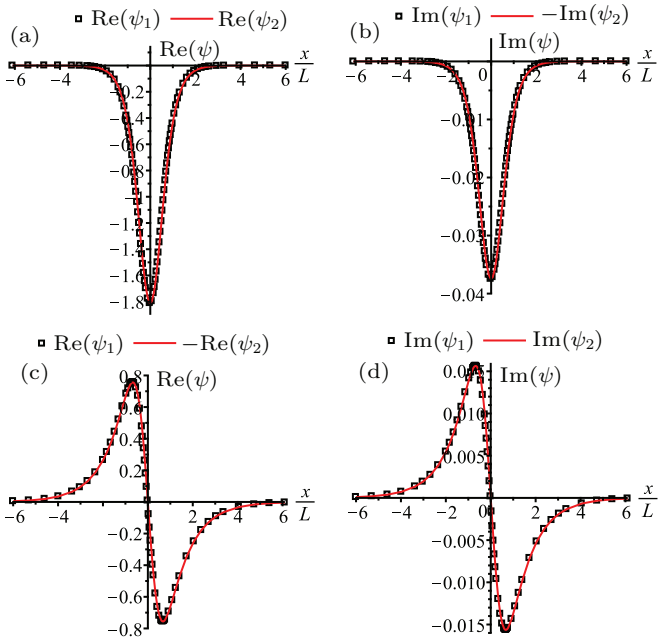


Fig. 3. Linear dependence between complex eigenfunctions $\psi_1(x/L)$ and $\psi_2(x/L)$ for the potential well $U_1(u=10)$. (a) Real part for $n=0$, (b) imaginary part for $n=0$, (c) real part for $n=1$, (d) imaginary part for $n=1$.

3. Exact solutions of potential well U_2

After substituting U_2 into Eq. (3) and taking the same variable y, we may rewrite Eq. (3) as

$$\begin{aligned}&(1-y^2)\frac{\mathrm{d}^2\psi(y)}{\mathrm{d}y^2}-2y\frac{\mathrm{d}\psi(y)}{\mathrm{d}y}\\&+\left[uy^2-\frac{m^2}{1-y^2}\right]\psi(y)=0.\end{aligned}\tag{25}$$

In a similar way to U_1, choosing the wave function of the form $\psi(y)=(1-y^2)^{m/2}\,\mathrm{e}^{\sqrt{u}y}F(y)$ and substituting it into above Eq. (25) yield the following differential equation for $F(y)$:

$$\begin{aligned}&(1-y^2)F''(y)+[2\sqrt{u}(1-y^2)-2(m+1)y]F'(y)\\&+[u-m(m+1)-2\sqrt{u}(m+1)y]F(y)=0.\end{aligned}\tag{26}$$

Through simple substitutions of variables $z=(1\mp y)/2$ into Eq. (26), we finally obtain two linearly dependent solutions $\psi_{1,2}(y)$ of Eq. (25) expressed by the confluent Heun functions

$$\begin{aligned}\psi_{1,2}(y)&=(1-y^2)^{m/2}\,\mathrm{e}^{\sqrt{u}y}\\&\times\mathrm{HeunC}\left(\mp4\sqrt{u},m,m,0,m^2/2-u,(1\mp y)/2\right).\end{aligned}\tag{27}$$

Substituting them into the Wronskian determinant (21) makes us obtain the following energy spectrum ε equation for potential well U_2

$$\begin{aligned}&\mathrm{HeunC}(-4\sqrt{u},m,m,0,m^2/2-u,1/2)\\&\times\mathrm{HeunCPrime}(4\sqrt{u},m,m,0,m^2/2-u,1/2)\\&+\mathrm{HeunC}(4\sqrt{u},m,m,0,m^2/2-u,1/2)\\&\times\mathrm{HeunCPrime}(-4\sqrt{u},m,m,0,m^2/2-u,1/2)=0.\end{aligned}\tag{28}$$

For $-0.25u<\varepsilon<0$, the intersections of $f(\varepsilon)$ with 'ε axis' as shown in Fig. 4

$$\begin{aligned}f(\varepsilon)\;=\;&\mathrm{HeunC}(-4\sqrt{u},m,m,0,m^2/2-u,1/2)\\&\times\mathrm{HeunCPrime}(4\sqrt{u},m,m,0,m^2/2-u,1/2)\\&+\mathrm{HeunC}(4\sqrt{u},m,m,0,m^2/2-u,1/2)\\&\times\mathrm{HeunCPrime}(-4\sqrt{u},m,m,0,m^2/2-u,1/2),\end{aligned}\tag{29}$$

determine the accurate eigenvalues ε and the number of bound states. Studying Eq. (29) enables us to decide how many the

bound states have (*i.e.* quantum number n) and the precise energy ε by using Maple. The results given in Table 2 are exactly same as those of Ref. [13]. Moreover, after substituting the calculated eigenvalues into Eq. (27) to perform the normalization operation, we find the following relation between them

$$N_1\psi_1(x/L) = (-1)^n N_2\psi_2(x/L), \tag{30}$$

which implies that they are linearly dependent (see Fig. 5).

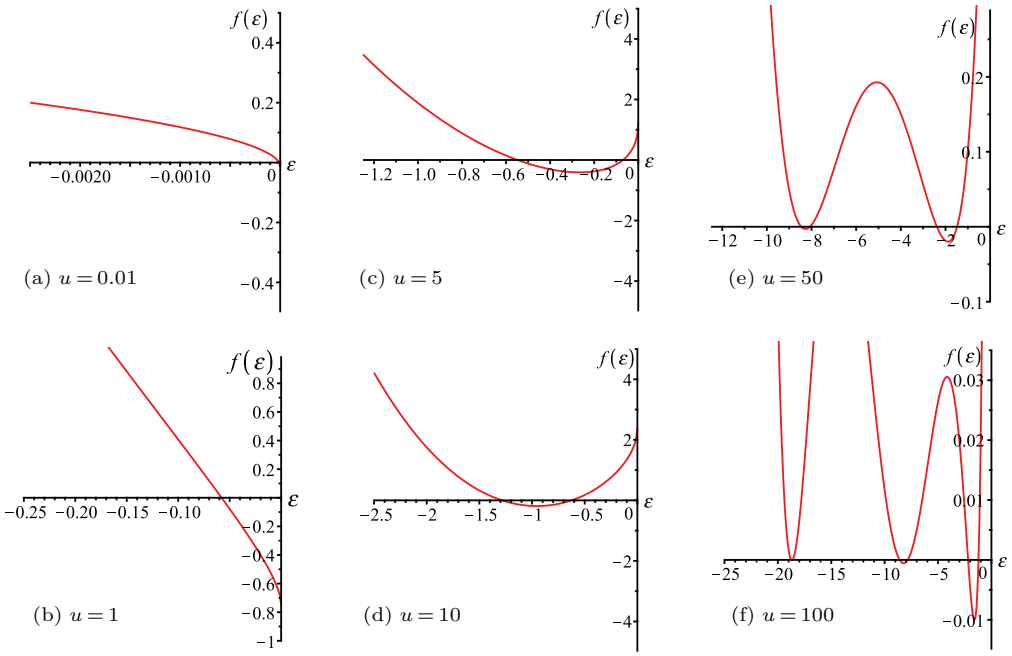


Fig. 4. Plot of $f(\varepsilon)$ as a function of ε with different depth u for the potential well U_2.

Table 2. Precise values of the dimensionless energy ε for potential well U_2.

n	$u=0.01$	$u=1$	$u=5$	$u=10$	$u=50$	$u=100$
	–0.0000 1100	–0.0578 4431	–0.5479 5221	–1.2842 5842	–8.4627 7461	–18.7641 4765
1			–0.0693 8127	–0.6258 5359	–8.0743 1992	–18.6169 0071
2					–2.3832 7594	–8.5956 5275
3					–1.4814 2123	–7.8396 0620
4						–2.1849 0137
5						–1.2085 3407

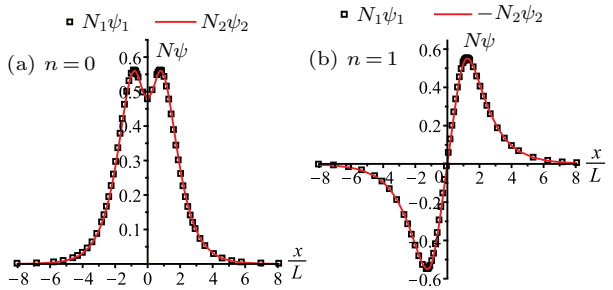


Fig. 5. Linear dependence between real eigenfunctions $\psi_1(x/L)$ and $\psi_2(x/L)$ for the potential well $U_2(u=10)$.

4. Exact solutions of potential well U_3

In a similar way to above, the corresponding Eq. (3) in this case becomes

$$(1-y^2)\frac{\mathrm{d}^2\psi(y)}{\mathrm{d}y^2} - 2y\frac{\mathrm{d}\psi(y)}{\mathrm{d}y} + \left[u + uy^2 - \frac{m^2}{1-y^2}\right]\psi(y) = 0. \tag{31}$$

The corresponding two linearly dependent solutions for this potential well are given by

$$\psi_{1,2}(y) = (1-y^2)^{m/2}\,\mathrm{e}^{\sqrt{u}y} \times \mathrm{HeunC}(\mp 4\sqrt{u}, m, m, 0, m^2/2 - 2u, (1\mp y)/2). \tag{32}$$

Let us define

$$\begin{aligned} f(\varepsilon) = {} & \mathrm{HeunC}(-4\sqrt{u}, m, m, 0, m^2/2 - 2u, 1/2) \\ & \times \mathrm{HeunCPrime}(4\sqrt{u}, m, m, 0, m^2/2 - 2u, 1/2) \\ & + \mathrm{HeunC}(4\sqrt{u}, m, m, 0, m^2/2 - 2u, 1/2) \\ & \times \mathrm{HeunCPrime}(-4\sqrt{u}, m, m, 0, m^2/2 - 2u, 1/2). \end{aligned} \tag{33}$$

to show its intersections with 'ε axis' for different depth u as illustrated in Fig. 6. The results are listed in Table 3. After substituting the eigenvalues, which is calculated by solving $f(\varepsilon)=0$, into Eq. (32), we find they satisfy the relation (30), which implies that they are linearly dependent as displayed in Fig. 7.

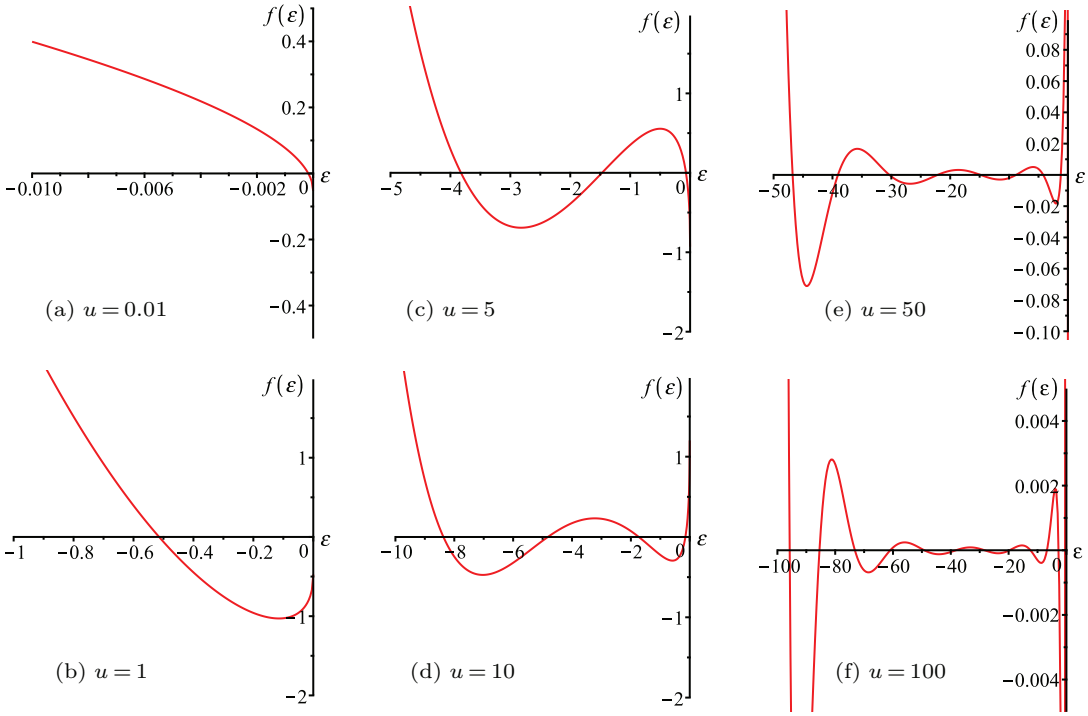


Fig. 6. Plot of $f(\varepsilon)$ as a function of ε with different depth u for the potential well U_3.

Table 3. Precise values of the dimensionless energy ε for the potential well U_3.

n	$u=0.01$	$u=1$	$u=5$	$u=10$	$u=50$	$u=100$
	–0.0001 7249	–0.5145 0970	–3.8235 1198	–8.3685 7941	–46.7708 3122	–95.7620 3281
1			–1.4702 6157	–4.8214 1046	–39.0686 6039	–85.4463 9269
2			–0.0682 4665	–1.7302 3961	–30.3256 4067	–73.1909 0670
3				–0.1464 6012	–22.1392 8916	–60.9528 9097
4					–14.8616 8162	–49.1765 3939
5					–8.8077 4240	–38.2217 6794
6					–4.1924 3631	–28.3269 6796
7					–1.2032 3602	–19.6803 9458
8					–0.0134 7079	–12.4372 0204
9						–6.7337 6967
10						–2.6959 0388
11						–0.4457 2570

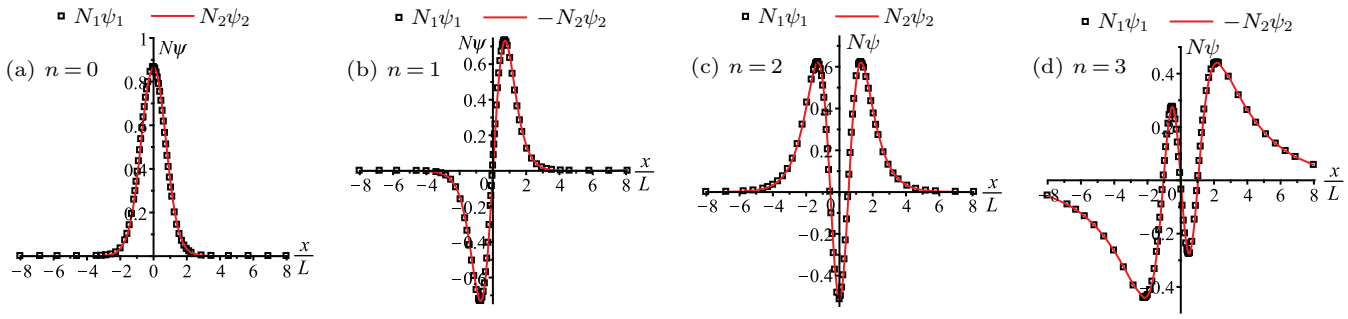


Fig. 7. Linear dependence between real eigenfunctions $\psi_1(x/L)$ and $\psi_2(x/L)$ for the potential well $U_3(u=10)$.

5. Conclusion

In this paper following the method used in our previous works,[29–33] we explored the exact solutions of the Schrödinger equation for a class of hyperbolic potential wells. This was realized by transforming the Schrödinger equation into a confluent Heun differential equation through using different forms of variable substitution and function transformation. And then two linearly dependent solutions for the same eigenstates were found to be used for constructing a Wronskian determinant, which leads to the energy spectrum equation. Then, the quantum number corresponding to each eigen-

state and the total number of bound states are graphically displayed. After that, we used Maple to calculate the exact energy ε of each eigenstate for different potential well U_q. Finally, the analytical wave function expressed by confluent Heun function can be gotten by substituting the obtained energy into the wave function. Before ending this work, we give two useful remarks on this method. In Ref. [15], when studying the hyperbolic potential well, the confluent Heun function satisfies two constraints,[15,34–36] (i) $\Delta_{N+1}(\mu)=0$, and (ii) $\mu+\nu+N\alpha=0$. The confluent Heun function will be truncated into an N degree polynomial to obtain the energy and the analytical wave function under special conditions. It is obvious to have some limitations to such an approach. This is because the second constraint (ii) cannot be satisfied for the present problem according to Eq. (11). As a result, the class of hyperbolic potential well studied here cannot be treated by the current method. It should be pointed out that the present method is especially suitable for symmetric regions with no singular points and no degeneracy of the eigenstates. In addition, the calculation of related functions in Maple may be not efficient for some special values, especially large parameters. We expect that this shortcoming will be improved as the version of Maple is updated.

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