On the quantum problem with harmonic, Stark, Coulombian and centrifugal barrier potential terms, and biconfluent Heun functions

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We show here that the one dimensional Schrödinger problem with a potential function with harmonic, Stark, Coulombian and centrifugal barrier terms can be described in terms of biconfluent Heun functions, and review some possible solutions of the problem. Considering the algebraic form of the quantum problem, we readily find two new relations between biconfluent Heun functions, which have not been considered before in the literature.

Keywords: Schrödinger equation; biconfluent Heun equation; exact solutions.

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1. Introduction

It is well known that there exist only a few exact solutions for the one dimensional time-independent Schrödinger equation,

$$-\frac{1}{2}\frac{d^2\psi(x)}{dx^2}+V(x)\psi(x)=E\psi(x), \tag{1}$$

(where we have used $\hbar$=m=1), and hence the class of solutions has been divided into two categories, exact and numerical. In the previous decades, a third class of problems appeared where only part of the spectrum could be found: some hyperbolic potentials, for example, led to this type of problems, where the appearance of the confluent Heun equation [1] is the relevant feature. This class of problems has introduced the so called quasi-exactly solvable (QES) potentials [2, 3].

Due to the relevance of the appearance of Heun equations, it is tempting to find out which Schrödinger problems may be solved using the different forms of Heun equations. In this sense, it is known that any second order linear differential equation with at most four singular points can be transformed into a Heun equation. The other Heun equations are its confluent, doubly confluent, biconfluent and triconfluent forms.

In particular, let us consider the biconfluent Heun (BCH) equation:

$$\frac{d^2y}{dz^2}+\left(\frac{\tilde{\gamma}}{z}+\tilde{\delta}+\tilde{\epsilon}z\right)\frac{dy}{dz}+\frac{\tilde{\alpha}z-\tilde{q}}{z}y=0, \tag{2}$$

which possess a regular singularity at $z=0$ and a rank-2 irregular singularity at $z=\infty$. Here, the parameters $(\tilde{\alpha},\tilde{\delta},\tilde{\gamma},\tilde{\epsilon},\tilde{q})\in\mathbb{C}^5$. The BCH functions have not been studied as much as the Heun or confluent Heun functions. As mentioned by Giscard and Tamar [4], there are no explicit integral series representation of Heun functions involving only elementary integrands, but some particular cases have been developed for each particular problem, as can be seen in the article by Vieira and Bezerra [5]. Here, owing to the solutions of our quantum problem, we shall present two new relations between BCH functions.

It is known that Eq. (2) can be written in terms of four irreducible parameters, its canonical form, the one mostly seen in physics articles [6], being

$$z\frac{d^2y}{dz^2}+\left(1+\alpha-\beta z-2z^2\right)\frac{dy}{dz}+\left[(\gamma-\alpha-2)z-\frac{1}{2}\left(\delta+(1+\alpha)\beta\right)\right]y=0\,. \tag{3}$$

where $(\alpha,\beta,\gamma,\delta)\in\mathbb{C}^4$. The parameters in Eq. (3) are related to those in Eq. (2) by

$$\tilde{q}=\frac{1}{2}\left[\delta+(1+\alpha)\beta\right],\ \tilde{\alpha}=\gamma-\alpha-2,$$
$$\tilde{\gamma}=1+\alpha,\ \tilde{\delta}=-\beta,\ \tilde{\epsilon}=-2. \tag{4}$$

Now, if we use

$$y(z)=z_0e^{-\frac{1}{2}z(\beta+z)}z^{\frac{1}{2}(1+\alpha)}\psi(z), \tag{5}$$

where z_0 may later be used as a normalization constant, we can get to the ordinary second order differential equation given by

$$-\frac{1}{2}\frac{d^2\psi}{dr^2}+\left[\frac{\alpha^2-1}{8}\frac{1}{r^2}+\frac{\delta k^{1/4}}{4}\frac{1}{r}+\frac{\beta k^{3/4}}{2}r+\frac{1}{2}kr^2\right]\psi=E\psi, \tag{6}$$

where r=$k^{-1/4}z$. Here we can recognize a Schrödinger problem with the potential function

$$V(r) = \frac{\alpha^2-1}{8}\frac{1}{r^2} + \frac{\delta k^{1/4}}{4}\frac{1}{r} + \frac{\beta k^{3/4}}{2} r + \frac{1}{2}kr^2, \qquad (7)$$

where the energy eigenvalue is

$$E = k^{1/2}\left(\frac{\gamma}{2} - \frac{\beta^2}{8}\right), \qquad (8)$$

and the constant k is used to resemble the harmonic oscillator potential term in Eq. (7). Due to transformation in Eq. (5), the problem is defined on the half-line, and, in order to have squared integrable functions for $z \in \mathbb{R}$, we must have $(\alpha, \beta) \in \mathbb{R}^2$, with $\alpha > -1$.

It is interesting to note that the energy eigenvalue is not proportional to the BCH equation eigenvalue in its canonical form, unlike, for example, the case of the quantum harmonic oscillator and Hermite's equation. Moreover, it is important to realize that the energy eigenvalues are essentially given by the parameter γ of the BCH equation.

2. The quantum problem

Let us now make the following identities:

$$\frac{1}{2}\beta k^{3/4} \equiv eD,\ \frac{1}{4}\delta k^{1/4} \equiv -e^2 Z,\ \alpha \equiv \pm(2\ell+1),$$

then we can write the potential function as

$$V(r) = \frac{1}{2}kr^2 + eDr - \frac{e^2 Z}{r} + \frac{\ell(\ell+1)}{2r^2}, \qquad (9)$$

which is a combination of harmonic, Stark, Coulomb and centrifugal-barrier potential terms. Notice that if ℓ is the angular momentum, the parameter α needs to be and odd integer.

This is a very interesting problem, from the point of view of quantum mechanics alone, since it includes potential terms from various exactly solvable problems, but that were not solved altogether exactly. Moreover, this problem actually appears in real chemical problems, as can be seen in the work of Karwowski and Witek [7].

From the derivation used, this is now a problem with known solutions, those of the BCH equation. The interesting question now is whether we can find exact solutions to this problem, or if only numerical solutions are possible.

2.1. The solutions

It has become a very important matter to study the BCH equation, and the BCH functions, due to its appearance in physical problems. For example, Ishkhanyan and Ishkhanyan present five cases where the BCH equation may be exactly solved in terms of Hermite polynomials [8]. In Ref. [9], Levai and Ishkhanyan present exact solutions of the sextic oscillator in terms of BCH functions, and in Ref. [10], Ferreira and Sesma find an algorithm to obtain solutions using a polynomial expansion, to cite a few examples. It is possible to find solutions for the eigenvalue problem (3) even if the problem is not related to physics, as shown in the work by John and Boyd [11]. As mentioned above, the lack of an explicit form for the BCH functions in terms of elementary series or elementary functions seems to have delayed the development of the understanding of the problems, but there exist now enough literature to work out specific cases. For the moment, let us take a closer look to a couple of solutions relevant to our current problem with the potential function in Eq. (7).

2.2. Solutions in terms of Hermite polynomials

In Ref. [8], Ishkhanyan and Ishkhanyan propose the following expansion of the solution of the BCH Eq. (2) in terms of the Hermite functions of a shifted and scaled argument:

$$y(z) = \sum_n c_n u_n\ ,\ u_n = H_{\alpha_0+n}\left(s_0(z+z_1)\right), \qquad (10)$$

where $(\alpha_0, s_0, z_1) \in \mathbb{C}^3$, and the Hermite functions satisfying the equation

$$\frac{d^2u_n}{dz^2} - 2s_0^2(z+z_1)\frac{du_n}{dz} + 2s_0^2\alpha_n u_n = 0,$$
$$\alpha_n = \alpha_0 + n, \qquad (11)$$

and the identities

$$u_n' = 2s_0\alpha_n u_{n-1}, \qquad (12)$$

$$s_0(z+z_1)u_n = \alpha_n u_{n-1} + u_{n-1}/2\,. \qquad (13)$$

In general, the index parameter α_0 is not an integer, so that the expansion functions are not reduced to polynomials or quasi-polynomials.

Upon substitution of Eqs. (10)-(11) into Eq. (2)], and using s_0=$\pm\sqrt{-\epsilon/2}$, $z_1 = \tilde{\delta}/\tilde{\epsilon}$, they get the three-term recurrence relation for coefficients c_n:

$$R_n c_n + Q_{n-1}c_{n-1} + P_{n-2}c_{n-2} = 0, \qquad (14)$$

where

$$R_n = \frac{\sqrt{2}}{\sqrt{-\epsilon}}(\alpha_0+n)\left(\tilde{\alpha} + (\alpha_0+n-\tilde{\gamma})\tilde{\epsilon}\right), \qquad (15)$$

$$Q_n = \mp\frac{\tilde{\alpha}\tilde{\delta} + (\tilde{q} + (\alpha_0+n)\tilde{\delta})\tilde{\epsilon}}{\tilde{\epsilon}}, \qquad (16)$$

$$P_n = \frac{\tilde{\alpha} + (\alpha_0+n)\tilde{\epsilon}}{\sqrt{-2\tilde{\epsilon}}}. \qquad (17)$$

The $\pm$ signs give different independent solutions, and the solution for physical applications is a linear combination of them.

For $\tilde{\epsilon} \neq 0$, with the initial conditions c_{-2}=c_{-1}=0, $c_0 \neq 0$, it is found that the series terminates at n=0, with R_0=0, if α_0=$\tilde{\gamma} - \tilde{\alpha}/\tilde{\epsilon}$. For the series to terminate at $n = N$, two successive coefficients have to vanish, c_{N+1}=c_{N+2}=0 while

$c_N \neq 0$. From equation c_{N+2}=0, the series ends if P_N=0. This condition is satisfied if $\tilde{\gamma}$=$-N$. The remaining equation, c_{N+1}=0, then renders a polynomial equation of degree $N+1$ for the parameter $\tilde{q}$, which defines, in general, $N+1$ values of $\tilde{q}$ for which the termination of the series occurs. These $N+1$ equations render then the corresponding physical solutions.

Ishkhanyan and Ishkhanyan then turn to give examples of potential functions for which this procedure works: in Ref. [8] they present five different cases where this work is applied, with the potential function in Eq. (9) being one of them.

Now, for the potential function in Eq. (9), we can see that we have that $\tilde{\epsilon} = -2$, which is in accordance to their work. However, we see that $\tilde{\gamma}$=$-N$, while from the parameter relations in Eq. (4), $\tilde{\gamma} = 1+\alpha$, giving $\alpha = -(N+1)$, and, since we have found that $\alpha = \pm(2\ell+1)$, the only possible choice is $\alpha = -2\ell - 1$. But then, we would have $1+\alpha < 0$, except for ℓ=0. Hence, $y(z)$ in Eq. (5) would become divergent at $z = 0$ for the case with $\tilde{\gamma}$=$-N$. This only means that the problem with the potential function in Eq. (9) does not possess solutions in terms of a series of Hermite polynomials if we have to relate the α parameter to the angular momentum. It seems that this divergence was not identified in Ref. [8].

Note, anyway, that the problem with a potential function with α not related to the angular momentum is anyway of great relevance. For example, one particular form has been studied for the description of quantum anomalies [12]. In that case, the potential function has an additional λ/r^2 term, but the Stark and harmonic terms are discarded.

2.3. Frobenius solutions

One other method of series solution for Eq. (6) is given by Ferreira and Sesma, [10] when α is not an integer, by first looking around the singularities at $r = 0$ and $r = \infty$. The algorithm description begins as follows:

For small r values, the series is given by

$$u_i(r) = \sum_{n=0}^{\infty} c_{n,i} r^{n+\nu_i}, \qquad i = 1, 2, \tag{18}$$

where

$$\nu_1 = \frac{1+\alpha}{2}, \qquad \nu_2 = \frac{1-\alpha}{2}, \qquad c_{0,i} = 1,$$

and the coefficients satisfying the three term recursion relation (3TRR)

$$n(n+2\nu_i - 1)c_{n,i} = \frac{\delta}{2} c_{n-1,i} - \left(\gamma - \frac{\beta^2}{4}\right) c_{n-2,i} + \beta c_{n-3,i} + c_{n-4,i}.$$

For large r, solutions are given in terms of Thomé solutions:

$$u_j(x) = e^{\sigma_j (x^2+\beta x)/2} x^{\mu_j} \sum_{m=0}^{\infty} a_{m,j} x^{-m}, \qquad j = 3, 4, \tag{19}$$

where

$$\sigma_3 = -1, \qquad \sigma_4 = 1, \qquad a_{0,j} = 1,$$
$$\mu_3 - (1-\gamma)/2, \qquad \mu_4 = -(1+\gamma)/2,$$

and the coefficients satisfying the 3TRR

$$2\sigma_j m a_{m,j} = -\left[\sigma_j \beta (m - 1 - \mu_j) + \frac{\delta}{2}\right] a_{m-1,j} + \left[(m-2-\mu_j)(m-1-\mu_j) + \frac{(1-\alpha^2)}{4}\right] a_{m-2,j}.$$

A global solution is found when there exist connection factors that bring $u_i(x)$ to $u_j(x)$, with i=1,2, j=3,4. This is achieved, for example, by using Naundorf's procedure [13]. In that case, the necessary combination for $x \to \infty$ is

$$u_i(x) \sim T_{i,3} u_3(x) + T_{i,4} u_4(x), \tag{20}$$

where $T_{i,j}$ are the connection factors

$$T_{i,3} = \frac{W[u_i, u_4]}{W[u_3, u_4]}, \qquad T_{i,4} = \frac{W[u_i, u_3]}{W[u_4, u_3]}, \tag{21}$$

with $W[u_i, u_j]$ the Wronskian between functions. This is not an easy task, and in Ref. [10] the authors introduce particular forms of the connecting functions that work for non-integer α.

For $\alpha > 1$, the solution regular at origin is

$$u_{reg}(x \to 0) = A_1 u_1(x), \tag{22}$$

while the solution regular at $x \to +\infty$ woud be

$$u_{reg}(x \to \infty) \sim A_1 T_{1,3} u_3(x), \tag{23}$$

with the requierement that $T_{1,4}$=0, and A_1 determined by the usual normalization condition. The complete algorithm, together with a numerical example, is found in Sec. 3 of [10].

Now, the problem is that the regular solutions are found only in the cases when α is not an integer [10]. This makes it difficult to apply the procedure for the case when α is related to the angular momentum. However, we may still find solutions for the problem with the potential function (7), with the condition α>-1, due to the transformation (5). We shall come back to the case $|\alpha|<1$ in the following section.

For the case of an eigenvalue problem, three of the four parameters $(\alpha, \beta, \gamma, \delta)$ are given, and the fourth is to be found. As one can see in the energy eigenvalue Eq. (8), this

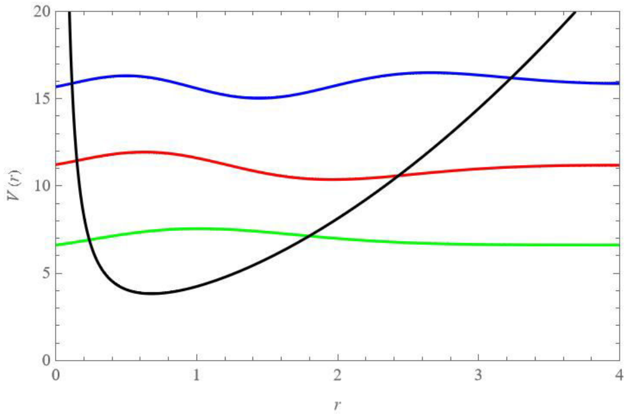

FIGURE 1. Potential function (black) and eigenfunctions for the problem (6) with $\alpha = 1.14$, $\beta = 1.5$ and $\delta = 2.2$.

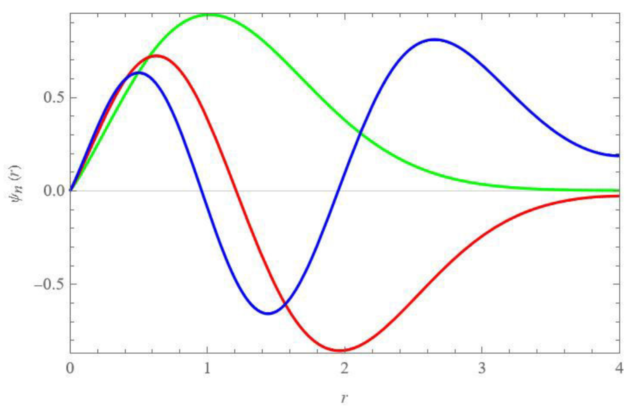

FIGURE 2. First three eigenfunctions for $\alpha = 1.14$, $\beta = 1.5$ and $\delta = 2.2$, for $n = 0$, in green, $n = 1$, in red, and $n = 2$, in blue.

parameter is γ, since the additional β^2 term may be added as a constant term in the potential function in Eq. (7), while γ does not appear anywhere else. There is not much work on this matter in the literature, to identify γ with the zeroes of the BCH function, but Arriola *et al.* have worked on the density of the zeros of BCH functions [14].

We may also solve the problem with the potential function in Eq. (7) numerically. For that matter, Mathematica [15] includes the defined function HeunB $(\tilde{q}_1, \tilde{\alpha}_1, \tilde{\gamma}_1, \tilde{\delta}_1, \tilde{\epsilon}_1; z)$. We reproduce here the example given in Ref. [10] using Mathematica to obtain the eigenvalues and eigenfunctions. We used

$$\alpha = 1.14, \quad \beta = 1.5, \quad \delta = 2.2,$$

and left the parameter γ, the eigenvalue, free. The first three values of γ found are

$$\gamma_1 = 6.6103, \quad \gamma_2 = 11.2199, \quad \gamma_3 = 15.6834.$$

Plots of the potential function, together with the eigenfunctions, are found in Fig. 1, and the eigenfunctions alone are shown in Fig. 2.

Being a useful academic tool, we give the Mathematica code used to obtain the eigenvalues and eigenfunctions in the Appendix.

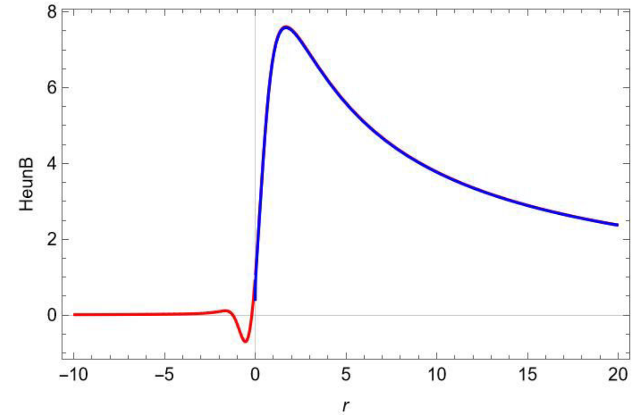

FIGURE 3. Mathematica's HeunB$(\tilde{q}_1, \tilde{\alpha}_1, \tilde{\gamma}_1, \tilde{\delta}_1, \tilde{\epsilon}_1; r)$ with $\tilde{q}_1 = 5$, $\tilde{\alpha}_1$=3.2, $\tilde{\gamma}_1$=0.8, $\tilde{\delta}_1 = 2$, and $\tilde{\epsilon}_1 = 4.1$ in red, and $1.8*$HeunB$(\tilde{q}_2, \tilde{\alpha}_2, \tilde{\gamma}_2, \tilde{\delta}_2, \tilde{\epsilon}_2; r)$, in blue. Due to the way Mathematica calculates fractional exponents, and the factor $r^{-\alpha}$, with $\alpha = -0.2$, Mathematica does not plot the blue curve for negative r.

3. New relations between BCH functions

Leaving aside the quantum problem, Eq. (6) may be useful to find some relations between BCH functions.

Firstly, we can see that Eq. (6) does not change when we replace α by $-\alpha$. Considering then the eigenfunction (5), we can see that the BCH functions of parameters $\pm\alpha$ are related by

$$H(-\alpha, \beta, \gamma, \delta; z) = z^{\alpha} H(\alpha, \beta, \gamma, \delta; z). \tag{24}$$

Since for the quatum problem we need that $\alpha > -1$, it may seem that this relation only holds for $|\alpha| < 1$. However, it is easily seen by direct substitution that it always holds for Eq. (3), and it is a general relation for BCH functions. A plot of the functions in both sides of Eq. (24) is found in Fig. 3, where a constant factor is used to superimpose the curves.

Secondly, we can see that Eq. (6) prevails after the following changes

$$x \to -x, \ \beta \to -\beta, \ \text{and}\ \delta \to -\delta\ .$$

Therefore, we get a second relation between BCH functions, given by

$$H(\alpha, -\beta, \gamma, -\delta; -z) = (-1)^{\frac{1+\alpha}{2}} H(\alpha, \beta, \gamma, \delta; z). \tag{25}$$

Plotting in terms of $z \in \mathbb{R}$, this means that there is a reflection along the $x-$axis if α is an odd-integer ($4n$+1, actually), as can be seen in Fig. 4, and solutions with α being an even-integer are not real. This is a feature that has been seen in physical problems, but was not completely understood. See, for example, the discussion in Sec. 6 of [10].

There seems to be no references for relations in Eqs. (24,25) in the literature. For example, Mathematica may find a general solution in terms of both of the functions in Eq. (24), not realizing they are the same.[i]

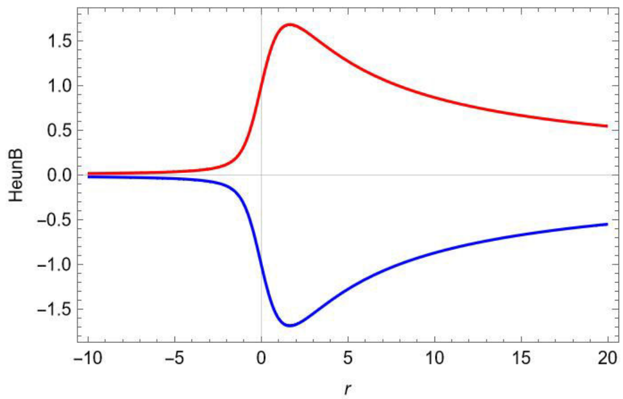

FIGURE 4. Mathematica's HeunB (5,3.2,6,2,4.1; r) in red, and HeunB (-5,3.2,6,-2,4.1; $-r$), in blue, where the change in the parameters is due to the change in β and δ as described in Eq. (25). A reflection along the x-axis is due to the factor $(-1)^{(1+\alpha)/2}$, in this case $\alpha = 5$.

4. Conclusion

Here we have made a review of solutions to the quantum problem with a potential function with harmonic, Stark, Coulombian and centrifugal barrier terms, which is essentially solved in terms of BCH functions. We have shown that this problem cannot be solved in terms of Hermite series, and provided the Mathematica code to obtain numerical solutions for this and other quantum problems.

Through this quantum problem we realized the existance of a new relation between BCH functions, where one parameter changed sign, and thereafter a second relation where the argument of the BCH functions changed sign, which may shed some light into the reality of the functions. We believe these relations have not been found anywhere else.

Finally, it would be interesting if, as one can see from Eq. (8), where the quantum energy eigenvalue is given in terms of the parameter γ of the BCH Eq. (2), there is a mathematical proof that when the BCH functions are determined as polynomials, the parameter γ is found to determine the zeroes of the BCH functions, a statement not settled yet in the literature.

Appendix A: Mathematica code

For the sake of academic purposes, we present here the Mathematica code used in Sec. 2.3 to solve the BCH Eq. (2) numerically:

```
In[168]:= a = 1.14; b = 1.5; d = 2.2;
h = 1;
m = 1;
V[x_] := (a^2 - 1) / (4 * x^2) + d / (2 * x) + (b / 2)^2 + b * x + x^2;
ℒ = - (h^2 / m) * u''[x] + V[x] * u[x];
{vals, funs} = NDEigensystem[ℒ, u[x], {x, 0, 4}, 3,
                 autovalores y autofunciones numéricas de operador diferencial
  Method →
  método
   {"SpatialDiscretization" →
     {"FiniteElement", {"MeshOptions" → {MaxCellMeasure → 0.0001}}}}];
                                         máxima medida de celda
vals
Show[Plot[Evaluate[h * funs + vals], {x, 0, 4}], Plot[V[x], {x, 0, 4}],
mue··· repr··· evalúa                             representación gráfica
 PlotRange → {{0, 4}, {0, 17}}, AxesOrigin → {0, 0}, ImageSize → Medium]
 rango de representación       origen de ejes      tamaño de i··· tamaño medio
Show[Plot[Evaluate[h * funs], {x, 0, 4}], PlotRange → {{0, 4}, {-0.8, 0.9}},
mue··· repr··· evalúa                     rango de representación
  AxesOrigin → {0, 0}, ImageSize → Medium]
  origen de ejes       tamaño de i··· tamaño medio
```

This code uses the parameter values for the example given by Ferreira and Sesma [10].

i. See reference.wolfram.com/language/ref/HeunB.html

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