# A MAPLE Symbolic-Numeric Program for Solving the 2D-Eigenvalue Problem by a Self-consistent Basis Method

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**Abstract.** The symbolic-numeric program SELFA for solving the the 2D boundary-value problem in self-consistent basis method is presented. The corresponding algorithm of this program using a conventional pseudocode is described too. As example, the energy spectrum and wave functions of E-type for generalized Henon–Heiles Hamiltonian were obtained.

## 1 Introduction

As is known, one of the more elaborated and widely applied methods of solving the eigenvalue problems describing the Hamiltonian systems is a diagonalization method [1]. However, in the case of multidimensional systems having a potential energy surface with few local minimuma[2], the efficiency of this method decreases in the energy region where in a classical limit a motion becomes chaotic [3]. An accuracy of numerical calculations of the corresponding set of energy levels of such type systems decreases drastically.

Usually one needs to diagonalize the Hamiltonian matrixes of a large dimension that leads to essential computer resource and run-time. In present paper the eigenvalue problem for a two-parametric generalized Henon–Heiles Hamiltonian corresponding to a non-integrable system is solved on the basis of a numerical method announced in [4]. In this method, the two-dimensional Schrödinger equation is reduced to a set of ordinary differential equations. Then the corresponding eigenvalue problem is solved directly instead of a rather cumbersome diagonalization of the above 2D problem. Such an approach is more promising due to an exact reduction by angular variable while numerical integration with a controlled accuracy is applied by a radial variable. This reduction is done with help of a self-consistent basis taking into account a discrete symmetry of the Hamiltonian under consideration that leads to a separation of the Hilbert space into the invariant subspaces and reduces the needed computer resources.

On the basis of this method we have developed the algorithm and MAPLE program SELFA for a symbolic-numeric solution of the two-dimensional Schrödinger equation. In this paper we give a unified description using a conventional pseudocode for the algorithm and program elaborated and present the energy spectrum and wave functions obtained by the program SELFA for a two-parametric generalized Henon–Heiles Hamiltonian.

## 2 Description of the Self-consistent Basis Method

We consider the stationary two-dimensional Schrödinger equation

$$\hat{H}(x,y)\psi(x,y) = E\psi(x,y), \tag{1}$$

with a two-parametric generalized Henon–Heiles Hamiltonian

$$\hat{H}(x,y) = -\frac{1}{2}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right) + \frac{1}{2}(x^2+y^2) + b(x^2 y - \frac{1}{3}y^3) + c(x^2+y^2)^2, \tag{2}$$

where $b$ and $c$ are the real-valued parameters. In a polar coordinate system, $x = r\cos\varphi$, $y = r\sin\varphi$, Eqs. (1) and (2) take the form

$$\hat{H}(r,\varphi)\psi(r,\varphi) = E\psi(r,\varphi), \tag{3}$$

$$\hat{H}(r,\varphi) = -\frac{1}{2}\left(\frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\frac{\partial^2}{\partial \varphi^2}\right) + \frac{r^2}{2} + \frac{br^3}{2}\sin 3\varphi + cr^4. \tag{4}$$

A regular and bounded solution of the partial eigenvalue problem for Eqs. (3)–(4) can be found in terms of the Fourier series

$$\psi(r,\varphi) = \frac{A_0(r)}{2\sqrt{r}} + \frac{1}{\sqrt{r}}\sum_{l=1}^{n}[A_l(r)\cos l\varphi + B_l(r)\sin l\varphi]. \tag{5}$$

Using the Galerkin projection of Hamiltonian $\hat{H}(r,\varphi)$ and the unknown solution $u(r,\varphi)$ onto basis functions, $\sin l'\varphi$ and $\cos l'\varphi$ ($l' = 0, ..., n$),

$$\frac{1}{\pi}\int_0^{2\pi} \cos l'\varphi \left(\hat{H}(r,\varphi) - E\right) u(r,\varphi) = 0, \tag{6a}$$

$$\frac{1}{\pi}\int_0^{2\pi} \sin l'\varphi \left(\hat{H}(r,\varphi) - E\right) u(r,\varphi) = 0, \tag{6b}$$

we obtain the following infinite system of the differential equations of the second order:

$$\begin{aligned}
&r^2 A_0'' + \alpha_0 A_0 - 2\beta B_3 = 0,\\
&r^2 A_1'' + \alpha_1 A_1 - \beta B_2 - \beta B_4 = 0,\\
&r^2 B_1'' + \alpha_1 B_1 - \beta A_2 + \beta A_4 = 0,\\
&r^2 A_2'' + \alpha_2 A_2 - \beta B_1 - \beta B_5 = 0,\\
&r^2 B_2'' + \alpha_2 B_2 - \beta A_1 + \beta A_5 = 0,\\
&r^2 A_3'' + \alpha_3 A_3 - \beta B_6 = 0,\\
&r^2 B_3'' + \alpha_3 B_3 - \beta A_0 + \beta A_6 = 0,\\
&r^2 A_l'' + \alpha_l A_l + \beta B_{l-3} - \beta B_{l+3} = 0, \qquad 4 \le l \le n,\\
&r^2 B_l'' + \alpha_l B_l - \beta A_{l-3} + \beta A_{l+3} = 0, \qquad A_{k>n} = B_{k>n} = 0.
\end{aligned} \tag{7}$$

Here parameters $\alpha_l$ and $\beta$ are defined by $\alpha_l = 2Er^2 - 2cr^6 - r^4 - l^2 + 1/4$, $\beta = br^5/3$. One can see that the system of equations (7) separates to four independent systems of the second-order ordinary linear differential equations (ODEs). This fact is a consequence of a discrete symmetry, $C_{3V}$, of the Henon–Heiles Hamiltonian (2) and corresponds to three irreducible representations:

$$\begin{array}{lllll} \mathrm{A}_1: & A_{6l}, & B_{6l+3}, & l = 0, 1, ..., & \\ \mathrm{A}_2: & B_{6l}, & A_{6l-3}, & l = 1, 2, ..., & \\ \mathrm{E}_1: & A_{6l+1}, & B_{6l+2}, & B_{6l+4}, & A_{6l+5}, \quad l = 0, 1, ..., \\ \mathrm{E}_2: & B_{6l+1}, & A_{6l+2}, & A_{6l+4}, & B_{6l+5}, \quad l = 0, 1, .... \end{array}$$

The E-type states of the type are double degeneracy because the eigenvalue problems for these two subsystems of the ODEs, ($\mathrm{E}_1$ and $\mathrm{E}_2$) have the same energy spectrum.

As an example, below we consider only $\mathrm{E}_2$-type states. Using an appropriate transformation

$$\begin{array}{llll} B_{6l+1} = z_{8l+1}, & B'_{6l+1} = z_{8l+2}, & A_{6l+2} = z_{8l+3}, & A'_{6l+2} = z_{8l+4}, \\ A_{6l+4} = z_{8l+5}, & A'_{6l+4} = z_{8l+6}, & B_{6l+5} = z_{8l+7}, & B'_{6l+5} = z_{8l+8}, \end{array}$$

of the above functions, $A_i(r)$, $B_j(r)$ $(i, j = 1, ..., n)$, to the new ones, $z_k(r)$ $r = 1, ..., 2N$, where $N$ is a number of equations of the ODEs of the second order, we rewrite the truncated set of linear second order ODEs ($\mathrm{E}_2$) in the form of the linear first order ODEs

$$\begin{array}{ll} {z_1}' - z_2 = 0, & {z_2}' + \alpha_1 z_1 - \beta(z_3 - z_5) = 0, \\ {z_3}' - z_4 = 0, & {z_4}' + \alpha_2 z_3 - \beta(z_1 - z_7) = 0, \\ {z_5}' - z_6 = 0, & {z_6}' + \alpha_4 z_5 + \beta(z_1 - z_9) = 0, \quad ... \ . \end{array} \tag{8}$$

To solve numerically the obtained eigenvalue problem one needs to reduce infinite interval $r \in (0, \infty)$ to a finite one $r \in [h, r_\infty]$, divide it by two subintervals, and construct the general solutions

$$\begin{array}{ll} z_j^0(r) = \sum\limits_{k=1}^{N} C_k z_{j,k}^0(r), & r \in [h, r_c], \\ z_j^\infty(r) = \sum\limits_{k=1}^{N} C_{k+N} z_{j,k}^\infty(r), & r \in [r_c, r_\infty]. \end{array} \tag{9}$$

Here $C_k$ are arbitrary coefficients and $z_{j,k}^0(r)$, $z_{j,k}^\infty(r)$, $j, k = 1, ..., 2N$ are independent basis solutions satisfying the set of equations (8) with boundary conditions,

$$z_{j,k}^0(h) = M_{j,k}^0, \quad z_{j,k}^\infty(r_\infty) = M_{j,k}^\infty, \tag{10}$$

where values $M_{j,k}^0$ and $M_{j,k}^\infty$ are determined from asymptotic expansions of regular solutions. Then, the continuity conditions

$$z_j^0(r_c) = z_j^\infty(r_c),$$

lead us to the algebraic eigenvalue problem

$$T_{jk} C_k = E_k C_k,$$

with a discrete spectrum $E_k$, i.e., at definite values of energy $E = E_s$ composing a low part of spectrum, $\sigma(E) = \{E_1, E_2, ..., E_N, ...\}$, of the eigenvalue problem (1)-(2).

## 3 Program Description

Following the description of the method for solving the eigenvalue problem (1)–(2), we present below the algorithm SELFA. The corresponding program SELFA has been implemented in a Maple Package.

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**Input:**
$N$ is the number of the second-order ordinary differential equations of the $E_2$ type;
$b,\ c$ are the real-valued parameters;
$h$ and $Rend$ are boundary points;
$r_c$ is a central point.
**Output:**
$\{E_s\}_{s=1}^{N}$ is a low part the energy spectrum;
$\{u_s(r,\phi)\}_{s=1}^{N}$ is the wave function corresponding to the energy value $E_s$ in a form of the Fourier series.
**The description of the local variables:**
$u(r,\phi)$ is the local function in a form of the Fourier series.
$V(x,y)$ and $V(r,\phi)$ is the Henon–Heiles potential function in Cartesian and polar coordinates;
$n$ is the number of the harmonics;
$A_k \equiv A_k(r),\ B_k \equiv B_k(r)$ $(k = 0, 1, ..., n)$ are the coefficients of the Fourier series;
$Baseq(r,\phi)$ is the l.h.s. of the basic equation $(\hat{H} - E)u = 0$ in polar coordinates;
$BaseqA_l, BaseqB_l$ are the l.h.s. of the second-order ODEs (7);
$Etype$ is the set of the second-order ODEs (7);
$z_j(r)$ are the unknown functions of the system of ODEs of the first order (8);
$ds$ are the l.h.s. of the first-order ODEs (8);
$dsys$ is the set of the first-order ODEs (8);
$M^0$ is the set of the initial conditions (10) on the left boundary for construction of sets of linear independent solutions of system of ODEs of the first order $dsys$;
$SOLN$ is the set of the linear independent solutions (9) of the set of the ODEs $dsys$;
$M^\infty$ is the set of values of the linear independent solutions (9) at the right boundary point $Rend$;
$T^0$, $T^\infty$ are the sets of values of the linear independent solutions (9) at the central point $r_c$;
$T$ is the matrix of the continuity conditions;
$\{C_j\}$ and $\{C_{j;s}\}$ are auxiliary eigenvectors;

**1:** $n := N + N/2 - 1;$

**2:** $u(r,\,\phi) := \dfrac{A_0}{2\sqrt{r}} + \dfrac{1}{\sqrt{r}} \sum_{k=1}^{n} (\, A_k \cos(k\,\phi) + B_k \sin(k\,\phi));$

**3:** $V(x,\,y) := \dfrac{1}{2}\,x^2 + \dfrac{1}{2}\,y^2 + b\,(x^2\,y - \dfrac{1}{3}\,y^3) + c\,(x^2 + y^2)^2;$

$V(r,\phi) := subs(x \to r\cos(\phi), y \to r\sin(\phi), V(x,y));$

**4:** $Baseq(r,\phi) := \left(\dfrac{1}{r^2}\dfrac{\partial^2}{\partial\phi^2} + 2(E + \dfrac{1}{8r^2} - V(r,\phi))\right) u(r,\phi);$

**for** $l$ **from** 0 **to** $n$ **do**

$BaseqA_l := r^2\text{coeff}(Baseq(r,\phi), \cos(l\phi));$

**if** $l \geq 1$ **then**

$BaseqB_l := r^2\text{coeff}(Baseq(r,\phi), \sin(l\phi));$

**end if**;

**end do**;

**5:** **for** $i$ **from** 0 **to** $(n+1)/6 - 1$ **do**

$Etype_{4i} := BaseqB_{6i+1};$

$Etype_{4i+1} := BaseqA_{6i+2};$

$Etype_{4i+2} := BaseqA_{6i+5};$

$Etype_{4i+3} := BaseqB_{6i+4};$

**end do**;

**for** $i$ **from** 0 **to** $N - 1$ **do**

**for** $j$ **from** 0 **to** $(n+1)/6 - 1$ **do**

$Etype_i := subs(\{B_{6j+1} \to z_{8j+1}(r), A_{6j+2} \to z_{8j+3}(r),$

$A_{6j+4} \to z_{8j+5}(r), B_{6j+5} \to z_{8j+7}(r)\}, Etype_i);$

**end do**;

**end do**;

**6:** **for** $i$ **from** 0 **to** $N - 1$ **do**

$ds_{2i+1} := \dfrac{dz_{2i+1}(r)}{dr} - z_{2i+2}(r) = 0;$

$ds_{2i+2} := \dfrac{dz_{2i+2}(r)}{dr} + \dfrac{Etype_i}{r^2} = 0;$

**end do**;

$dsys := \{ds_1, ds_2, ..., ds_{2N}\};$

**7:** **for** $i$ **from** 1 **to** $N$ **do**

$SOLN := dsolve(\{dsys, z_j(h) = M^0_{i,j}, (j = 1, ..., 2N)\}, \{z_j(r)\}_{j=1}^{2N});$

$T^0_{ij} := SOLN : z_j(r_c), \quad (j = 1, ..., 2N);$

$SOLN := dsolve(\{dsys, z_j(Rend) = M^\infty_{i,j}, (j = 1, ..., 2N)\}, \{z_j(r)\}_{j=1}^{2N});$

$T^\infty_{ij} := SOLN : z_j(r_c), \quad (j = 1, ..., 2N);$

**end do;**

**8:** **for** $i$ **from** 1 **to** $N$ **do**

**for** $j$ **from** 1 **to** $2N$ **do**

$T_{ij} := T^\infty_{ij} - T^0_{ij};$

**end do**;

**end do**;

**9:** $T_{ij}C_j = EC_j \quad \to \quad \{E_s, \{C_{j;s}\}\}_{s=1}^{N}$

**10:** **for** $s$ **from** 1 **to** $N$ **do**

$SOLN_s := dsolve(\{dsys, z_j(h) = C_{j;s}, (j = 1, ..., 2N)\}, \{z_j(r)\}_{j=1}^{2N})$;
$u_s(r, \phi) := SOLN_s :$
$\sum_{j=0}^{(n+1)/6-1}\Big(z_{8j+3}(r)\cos((6j+2)\phi) + z_{8j+5}(r)\cos((6j+4)\phi)$
$+z_{8j+1}(r)\sin((6j+1)\phi) + z_{8j+7}(r)\sin((6j+5)\phi)\Big)$;

**end do;**

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**Remark:** This program involves the following sequence of the steps.
Steps 1–2. The wave function in the form of the Fourier series is presented.
Steps 3–4. Construction of the set of the second-order ODEs. At step 4 instead of formula (6) the standard MAPLE procedure "coeff" for extracting coefficients affecting $\cos(l\phi)$ and $\sin(l\phi)$ is used.
Steps 5–6. Construction of the set of the first-order ODEs.
Step 7. Construction of the linear independent solutions with help of the conventional subroutine *dsolve* of a Maple package for numerical solving of a set of the $2N$ first order ODEs.
Step 8. Construction of continuity conditions matrix.
Step 9. Evaluation of the energy spectrum.
Step 10. Evaluation of the eigenfunctions.

## 4 Examples of SELFA Program Runs

The eigenvalues and functions of $E_2$-types were calculated by means of the program SELFA for a generalized Henon–Heiles Hamiltonian. Values of the lowest energy levels together with the ones obtained by the diagonalization method [5] are presented in Table 1. The energy spectrum in Ref. [5] was obtained by a direct diagonalization of the Hamiltonian $495 \times 495$ matrix but in our approach the same accuracy was achieved by solving system (8) of $2N = 16$ differential equations of the first order. It is shown that in our approach one needs a less computer resource and running time in comparison with the diagonalization method. The program SELFA was also used to calculate the corresponding wave functions, two of which are shown in Fig. 1. One can see that a symmetric struc-

**Table 1.** The energy spectrum of E-type for the Hamiltonian (2) at fixed values of parameters $b = 0.04416$, $c = 0.00015$

| s | $E_{diag}$[4] | $E$ | $s$ | $E_{diag}$[4] | $E$ |
|---|---|---|---|---|---|
| 1. | 1.999384 | 1.999372 | 7. | 6.005955 | 6.005972 |
| 2. | 2.999628 | 2.999641 | 8. | 6.976317 | 6.976625 |
| 3. | 3.992368 | 3.992439 | 9. | 6.988910 | 6.989034 |
| 4. | 4.990280 | 4.990394 | 10. | 7.964477 | 7.964810 |
| 5. | 5.002921 | 5.002935 | 11. | 7.989611 | 7.989745 |
| 6. | 5.980721 | 5.980968 | 12. | 8.014769 | 8.014855 |

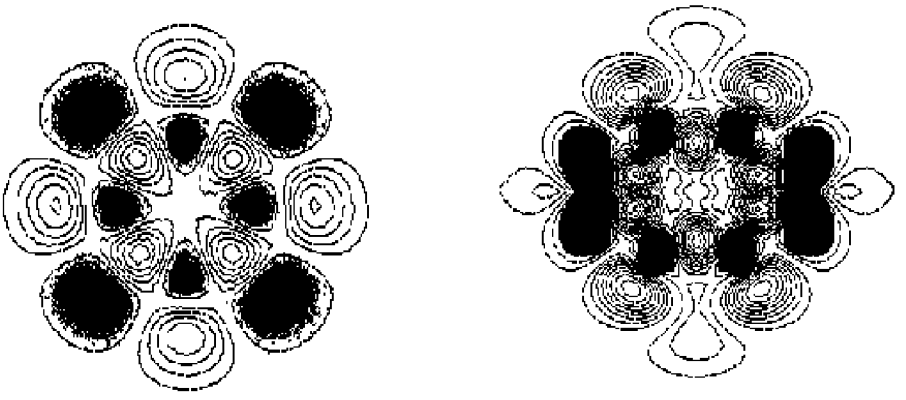

**Fig. 1.** Isolines of the $E_2$-type wave functions $u_9(x, y)$ (in left panel) and $u_{11}(x, y)$ (in right panel) of the generalized Henon–Heiles Hamiltonian (2) at $b = 4.416 \cdot 10^{-2}$ and $c = 1.5 \cdot 10^{-4}$ (dark and white domains correspond to negative and positive values, respectively)

ture of isolines of the wave functions $u_9(x, y)$ and $u_{11}(x, y)$ reveals explicitly the $C_{3V}$ symmetry of the generalized Henon–Heiles Hamiltonian (2).

## 5 Conclusions

A MAPLE program SELFA for a symbolic-numeric solution of the two-dimensional Schrödinger equation in self-consistent basis method is presented. An efficiency of this program is shown on an example of the generalized Henon–Heiles Hamiltonian (2) for which the lowest energy levels and wave functions were calculated and a comparison was made with the results obtained by diagonalization method. The program SELFA may further be applied for studying the eigenproblem for different Hamilton operators and, for example, for investigating the avoiding crossing phenomena of eigenenergies, etc.

One of topical tasks here is a comparison of numeric and analytic results for spectrum and wave functions in a vicinity of avoiding crossing of energy levels with respect to parameters that can be performed with help of the above algorithm SELFA and programs of normalization and quantization of the polynomial Hamiltonians [6,7]. Such a comparison allows one to reveal the nature of quantum chaos of the Hamiltonian systems that in quantum case has quantum counterparts like a degeneracy of the energy levels and tunnelling through a potential barrier with few local extrema and to determine various decay mechanisms of the quantum system under consideration. A study in the field will be a subject of our further investigations.

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