A Symbolic-Numeric Approach for Solving the Eigenvalue Problem for the One-Dimensional Schrödinger Equation

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Abstract. A general scheme of a symbolic-numeric approach for solving the eigenvalue problem for the one-dimensional Shrödinger equation is presented. The corresponding algorithm of the developed program EWA using a conventional pseudocode is described too. With the help of this program the energy spectra and the wave functions for some Schrödinger operators such as quartic, sextic, octic anharmonic oscillators including the quartic oscillator with double well are calculated.

1 Introduction

For solving a stationary Shrödinger equation a lot of approximate analytical and numerical methods are elaborated and applied because an exact solution in explicit form exists only for some specific hamiltonians [1]. As is known, the more used methods are diagonalization [2, 3], quasiclassical approach [4], continuous analogue of Newton's method [5], different versions of perturbation theory [6], normal form method [7, 8, 9, 10, 11], finite-element method [12], $1/N$ expansion [13], oscillator representation [14], variational and operational methods [15, 16, 17], simplectic method [18] and etc.

The method of integration by means of the power series is known to be a simple one but it requires cumbersome work, and difficulties are increasing in the cases when a differential equation has singularities[19]. On the other hand, an application of the modern PC together with packages of symbolic manipulations such as MAPLE, MATHEMATICA, REDUCE enable us to carry out necessary calculations and construct the solution of differential equation in the form of power series up to a desired degree.

In the present work, an analytic numeric approach for solving the time independent Shrödinger equation is proposed. The developed method is based on finding a general solution as a sum of two independent solutions.

By this method the spectra and wave functions for a quartic, sextic, and octic anharmonic oscillators and also for the quartic oscillator with two minima were calculated. Obtained results are in good agreement with the ones available in literature.

2 General Scheme of the Method

Let us consider the eigenvalue problem for ordinary differential equation

$$\frac{d^2\psi(x)}{dx^2} + 2(E - V(x))\Psi(x) = 0, \tag{1}$$

where the function $V(x)$ can have a pole not above the second order in a vicinity of the point x_0, and independent variable x belong to the real axis or semiaxis.

For fixed value of E differential equation (1) has two linear independent solutions $y_1(x)$ and $y_2(x)$. If the function $V(x)$ is regular at point $x = x_0$ we find $y_1(x)$ and $y_2(x)$ as solutions of Cauchy problem (1) with boundary conditions

$$y_1(x_0) = 1, \quad \left.\frac{dy_1(x)}{dx}\right|_{x=x_0} = 0, \quad y_2(x_0) = 0, \quad \left.\frac{dy_2(x)}{dx}\right|_{x=x_0} = 1 \tag{2}$$

in the form of Taylor series

$$y_1(x) = 1 + \sum_{k=2}^{N} c_k^{(1)}(x - x_0)^k, \quad y_2(x) = (x - x_0) + \sum_{k=2}^{N} c_k^{(2)}(x - x_0)^k. \tag{3}$$

Substituting (3) into (1) we obtain recurrence relations for evaluation of coefficients $c_k^{(1)}$ and $c_k^{(2)}$.

If the function $V(x)$ has a pole of order not higher than the second, i.e.

$$2(E - V(x)) = (x - x_0)^{-2} \sum_{k=0}^{N} f_k(x - x_0)^k,$$

the solutions of (1) will be found in form of generalized power series

$$y(x) = (x - x_0)^{\rho} \sum_{k=0}^{N} c_k(x - x_0)^k. \tag{4}$$

Substituting (4) into (1) we find determining equation

$$\rho(\rho - 1) - f_0 = 0. \tag{5}$$

It is known from the theory of ordinary differential equations [23] that the form of independent solutions depends on the roots ρ_1 and ρ_2 of Eq. (5).

1. If the difference of roots, $\rho_1 - \rho_2$ is not equal to an integer, then two linear independent solutions can be present in the form

$$y_1(x) = (x - x_0)^{\rho_1} \sum_{k=0}^{N} c_k^{(1)}(x - x_0)^k, \tag{6}$$

$$y_2(x) = (x - x_0)^{\rho_2} \sum_{k=0}^{N} c_k^{(2)}(x - x_0)^k.$$

2. If the difference of roots, $\rho_1 - \rho_2$ is equal to an integer, then two linear independent solutions can be present in the form

$$y_1(x) = (x - x_0)^{\rho_1} \sum_{k=0}^{N} c_k^{(1)} (x - x_0)^k, \tag{7}$$

$$y_2(x) = (x - x_0)^{\rho_2} \sum_{k=0}^{N} c_k^{(2)} (x - x_0)^k + \xi_{-1} y_1(x) \ln(x - x_0),$$

where $\rho_1 > \rho_2$.

In these two cases we also find the recurrence relations for coefficients $c_k^{(1)}$, $c_k^{(2)}$ by substitution of expansion (6) or (7) into differential equation (1).

The general solution of Eq. (1) takes the form

$$\psi(x) = C_1 y_1(x) + C_2 y_2(x). \tag{8}$$

In physical applications, one needs to find bounded solutions, therefore, we truncate an infinite interval to a finite one $x \in (R_{left}, R_{right})$ and supply the following boundary conditions

$$\psi(R_{left}) = 0, \quad \psi(R_{right}) = 0. \tag{9}$$

Then coefficients C_1 and C_2 satisfy the set of homogeneous algebraic equations

$$C_1 y_1(R_{left}) + C_2 y_2(R_{left}) = 0, \quad C_1 y_1(R_{right}) + C_2 y_2(R_{right}) = 0. \tag{10}$$

A nontrivial solution of system (10) is found from condition of equality to zero of determinant

$$D(E) = \begin{vmatrix} y_1(R_{left}) & y_2(R_{left}) \\ y_1(R_{right}) & y_2(R_{right}) \end{vmatrix} = 0, \tag{11}$$

which is carried out at certain values of energy making an energy spectrum $E = \{E_k\}$ of Schrödinger equation (1). For given $E = E_k$, the coefficients C_1 and C_2 are calculated from Eq. (10), including an additional normalization condition

$$\int_{R_{left}}^{R_{right}} |\psi(x)|^2 dx = 1 \tag{12}$$

for the wave function (8).

3 Description of the Program

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

Input:
$V(x)$ is potential;
R_{left} and R_{right} are bounds of a truncated interval of the independent variable x;
N is the number of terms of the power series;
Output:
$\{E_k\}$ and $\{\psi_k(x)\}$ are set of energy levels and wave functions of the equation (1);
The description of the local variables:
TypeV is the flag, if TypeV=0 then $V(x)$ does not have singularity in x_0, if TypeV=1 then $V(x)$ has a pole in x_0;
$c_k^{(1)}$ and $c_k^{(2)}$ are coefficients of the two linear independent solutions of the equation (1);
ρ_1, ρ_2 are the solutions of the determining equation (5);
ξ_{-1} is a coefficient in expansion (7);
$y_{1,2}(R_{left})$, $y_{1,2}(R_{right})$ are values of two linear independent solutions in bounds of interval;
C_1 and C_2 are auxiliary coefficients;

1: $V(x), x_0 \quad \rightarrow \quad TypeV$;
2: if TypeV=0 then
2.1: $y_1(x) \rightarrow 1 + \sum_{k=2}^{N} c_k^{(1)} (x - x_0)^k$;
2.2: $y_2(x) \rightarrow (x - x_0) + \sum_{k=2}^{N} c_k^{(2)} (x - x_0)^k$;
3: else if TypeV=1 then
3.1: $\rho(\rho - 1) - f_0 = 0 \quad \rightarrow \quad \rho_1,\ \rho_2$;
3.2: $y_1(x) \rightarrow (x - x_0)^{\rho_1} \sum_{k=0}^{N} c_k^{(1)} (x - x_0)^k$;
3.3: $y_2(x) \rightarrow (x - x_0)^{\rho_2} \sum_{k=0}^{N} c_k^{(2)} (x - x_0)^k + \xi_{-1} y_1(x) \ln(x - x_0)$;
end if
4: $C_1 y_1(R_{left}) + C_2 y_2(R_{left}) = 0,$
$C_1 y_1(R_{right}) + C_2 y_2(R_{right}) = 0, \quad \rightarrow \quad E_k$;
5: E_k + normalization conditions $\quad \rightarrow \quad C_1,\ C_2 \quad \rightarrow \quad \psi_k(x)$

Remark: This program involves the following sequence of steps.
Step 1. Determination of value of flag TypeV.
Step 2. Finding two linear independent solutions if the potential function $V(x)$ does not have a pole.
Step 3. The coefficients ρ_1, ρ_2, $c_k^{(1)}$, $c_k^{(2)}$ and ξ_{-1} of expansion (3) for regular potential, or (6), (7) depending on the result of the solution for the determining equation (5) for singular potential, are evaluated. At this step, the coefficients $c_k^{(1)}$, $c_k^{(2)}$, and ξ_{-1} depend on E explicitly.
Step 4. Evaluation of the energy spectrum from boundary conditions (10).
Step 5. Evaluation of the eigenfunctions using normalization conditions.

Table 1. The comparison of energy levels E_{EWA} with their exact values E_{exact} (14) for $l = 1, 2, 3$ ($R_{left} = 10^{-8}$, $R_{right} = 5.6$, $N = 116$, $\varepsilon = |E_{EWA} - E_{exact}|/E_{exact}$)

$l = 1$			
n	E_{EWA}	E_{exact}	$\varepsilon, \%$
0	2.00000000044	2	0.0000000022
1	4.000000017	4	0.00000043
2	6.0000020	6	0.000033
3	8.000083	8	0.0010
$l = 2$			
n	E_{EWA}	E_{exact}	$\varepsilon, \%$
0	3.00000000066	3	0.000000022
1	5.00000016	5	0.0000032
2	7.000013	7	0.00018
3	9.00037	9	0.0041
$l = 3$			
n	E_{EWA}	E_{exact}	$\varepsilon, \%$
0	4.0000000067	4	0.00000016
1	6.0000011	6	0.000018
2	8.000066	8	0.00082
3	10.0013	10	0.013

4 Examples of the EWA Program Runs

To test the EWA program the one-dimensional (1) and radial Shrödinger equations were considered with the potential functions such that solutions are known:
A) infinite rectangular wall $V(x) = \{0, |x| \le R; \infty, |x| > R\}$;
B) harmonic oscillator $V(x) = x^2/2$;
C) the two-dimensional axial symmetric harmonic oscillator $V(r) = 1/2\omega r^2$ (in this case we use r instead of x).

In case A), ten lowest energy levels coincide with exact $E_n = \pi^2 n^2/8R^2, \quad n = 1, ...10, ...$ to nine significant figure accuracy if $N = 68$ and $R_{left} = -R$, $R_{right} = R$, $R = 1$.

In case B), for $x \in [R_{left}, R_{right}]$ ($-R_{left} = R_{right} = R = 5.9$, $N = 138$) the accuracy ε of the 10th energy level obtained is less than 0.004% compared with exact value $E_{10} = 10.5$. And absolute difference between calculated and exact wave function $|\psi_{EWA} - \psi_{exact}|$ is less than 10^{-9}. Note, the accuracy depends on values of R and N, and its magnitude may be increased.

In case C), for $\omega = 1$ the differential equation on the semiaxis $r \in [0, \infty)$

$$\frac{d^2y(r)}{dr^2} + \left(2E + \frac{1 - 4l^2}{4r^2} - r^2\right)y(r) = 0, \tag{13}$$

has the double pole in origin, and its eigenvalues and functions are known [20]

$$E_n = 2n + |l| + 1, \; n = 0, 1, 2, \ldots, \quad l = 0, \pm 1, \pm 2, \ldots \tag{14}$$

Table 2. The comparison of energy levels $2E_{EWA}$ with their values E_{exact} from [3] for different powers μ ($\alpha = 0.0005$ for $\mu = 4, 6$ and $\alpha = 0.00005$ for $\mu = 8$)

	$\mu = 4$,	$R_{left} = -5.6$, $R_{right} = 5.6$,	$N = 116$
n	$2E_{EWA}$	E_{exact}	ε
0	1.0007486926734	1.00074869267319	0.000000000019
1	3.00373974818	3.00373974816873	0.00000000046
2	5.009711873	5.00971187278811	0.0000000080
3	7.018652599	7.01865259205752	0.00000010
4	9.0305496	9.03054956607471	0.0000011
5	11.045391	11.0453905781793	0.0000094
6	13.06317	13.0631635776785	0.000065
7	15.0839	15.0838565876260	0.00043
8	17.1078	17.1074577926535	0.0022
9	19.134	19.1339554918523	0.0031
10	21.164	21.1633381057038	0.0060
	$\mu = 6$,	$R_{left} = -4.7$, $R_{right} = 4.7$,	$N = 116$
n	$2E_{EWA}$	E_{exact}	ε
0	1.001848816	1.0018488155723	0.000000045
1	3.01278097	3.0127809606901	0.00000056
2	5.0448002	5.0447999257845	0.0000060
3	7.110096	7.1100928558609	0.000048
4	9.21860	9.2185817487322	0.00030
5	11.3779	11.377808617207	0.0015
	$\mu = 8$,	$R_{left} = -4.6$, $R_{right} = 4.6$,	$N = 108$
n	$2E_{EWA}$	E_{exact}	ε
0	1.00064637	1.0006463698740	0.00000012
1	3.00572693	3.0057269553512	0.00000070
2	5.0253946	5.0253949690878	0.0000061
3	7.07668	7.0766689726027	0.00016
4	9.18033	9.1802567401069	0.00088
5	11.3565	11.356154413293	0.0038

$$y_{nl}(r) = (-1)^n \sqrt{\frac{2n!}{(n+l)!}} \exp(-\frac{r^2}{2}) \cdot r^{l+\frac{1}{2}} \cdot L_n^{(l)}(r^2), \tag{15}$$

where $L_n^{(l)}(r^2)$ are the Chebyshev–Laguerre polynomials. For equation (13), the eigenfunctions and the energy spectrum were found with the help of the program EWA. A comparison of the calculated and exact eigenvalues for different values of l is presented in Table 1. As an example, we present the series expansion of two linear independent solutions of equation (13) at point $r = 0$ for $l = 1$ and $N = 8$:

$$y_1(r) = r^{\frac{3}{2}} \left(1 - \frac{Er^2}{4} + \frac{(E^2+2)r^4}{48} - \frac{(E^3+8E)r^6}{1152} + \frac{(E^4+20E^2+24)r^8}{46080}\right),$$

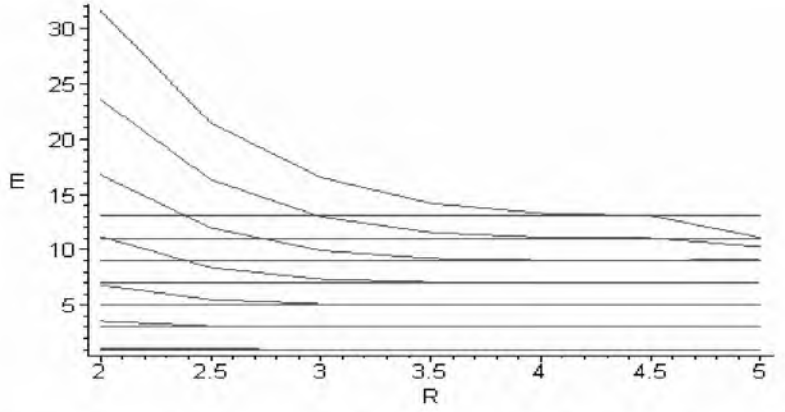

Fig. 1. The evaluated energy levels E_k,$k = 1, ..., 7$ of anharmonic oscillator with potential (16) versus the boundary point R for $\mu = 4$, $\alpha = 1$, and $N = 72$. Exact values E_k^{exact} are shown by straight lines.

$$y_2(r) = r^{-\frac{1}{2}} \left(-\frac{1}{2} + \frac{Er^2}{8} - \frac{(1-E^2)r^4}{16} + \frac{(2E-11E^3)r^6}{1152} \right) + \frac{E}{2} y_1(r) \ln r.$$

4.1 Quartic, Sextic, and Octic Anharmonic Oscillators

The above presented method has been applied for calculation of energy levels and wave functions of anharmonic oscillator with nonlinearity of the fourth, sixth, and eighth degrees so that potential functions $V(x)$ have the following forms

$$V(x) = \frac{x^2}{2} + \alpha x^{\mu}, \quad \mu = 4, 6, 8, \tag{16}$$

where $\alpha > 0$ is parameter of nonlinearity. Using EWA program for Shrödinger equation (1) with potential functions (16) the energy spectra and wave functions in the form of power series were found. The calculated energy levels are present in Table 2. The behaviour of determinant $D(E)$, and, hence, of roots $\{E_k\}$ of equation (10) strongly depends on the number of terms N in power series (7) and on the value of $R = -R_{left} = R_{right}$. As N increases the values of roots of equation (10) come nearer to true values if as necessary to increase the value of R. In Fig. 1, the energy values are shown at fixed N versus the R value.

4.2 Anharmonic Oscillator with Two Minima

The potential function of anharmonic oscillator with two minima takes form

$$V(x) = \alpha(x^2 - a^2)^2. \tag{17}$$

Here $\alpha > 0$ is parameter of nonlinearity, and a is parameter that determine the position of two minima of potential function (17). In this case wave functions

Table 3. The comparison of energy levels $2E_{EWA}$ of potential function (17) with their values $2E_J$ from [15]

$a=\sqrt{2}$, $\alpha=1$, $R_{left}=-3.4$, $R_{right}=3.4$, $N=180$		
n E_{EWA}	E_J	ε
0 1.80081349	1.80081349	0
1 1.89650538	1.89650538	0
2 4.37046673	4.37046673	0
3 5.57335024	5.5733520	0.0000007
4 7.65142527	-	-
5 9.92036057	-	-

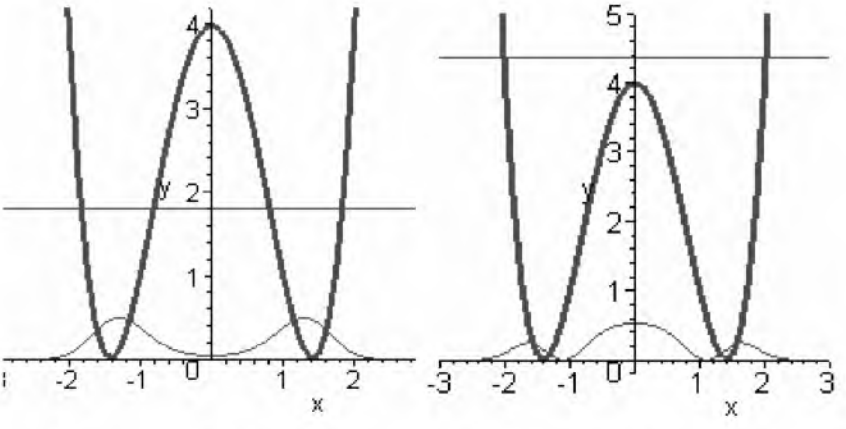

Fig. 2. The square of wave function, $|\Psi(x)|^2$ of the ground state (left panel) and for state with $n=2$ (right panel). The thick lines is the potential function $V(x)$.

and energy spectrum for Schrödinger equation (1) were also calculated by means of the program EWA for different values of parameters a and α. As an example, we show the series expansion of two linear independent solutions at point $x=0$ for $N=7$:

$$y_1(x) = 1 + (\alpha a^4 - E)x^2 + \frac{1}{6}\left(E^2 - 2E\alpha a^4 + \alpha^2 a^8 - 2\alpha a^2\right)x^4$$
$$+\frac{1}{90}\left(-E^3 + 3E^2\alpha a^4 - 3E\alpha^2 a^8 + 14E\alpha a^2 + \alpha^3 a^{12} - 14\alpha^2 a^6 + 6\alpha\right)x^6,$$
$$y_2(x) = x + \frac{1}{3}\left(\alpha a^4 - E\right)x^3 + \frac{1}{30}\left(E^2 - 2E\alpha a^4 + \alpha^2 a^8 - 6\alpha a^2\right)x^5,$$
$$+\frac{1}{630}\left(-E^3 + 3E^2\alpha a^4 - 3E\alpha^2 a^8 + 26E\alpha a^2 + \alpha^3 a^{12} - 26\alpha^2 a^6 + 20\alpha\right)x^7.$$

The values of lowest energy levels and plots of wave functions are presented in Table 3 and in Fig. 2.

Acknowledgments

Authors are deeply indebted to Prof. I.V. Puzynin and to the participants of his seminar for a useful discussion. This work is partially supported by BelSU (grant VKG-003-04).

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