METHOD FOR THE NUMERICAL SOLUTION OF THE STATIONARY SCHRODINGER EQUATION

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ABSTRACT

A general method for numerical solution of eigenfunction problems is presented. The method is based on differential T-transform technique and the acceleration properties of the Padé approximation. The advantages of the method consist in its quick-action and the possibility to find precisely the searching solution, especially in cases when the conventional methods do not work. Mathieu's eigenfunctions at extremely high q-parameter are obtained in order to illustrate the power of the method.

KEYWORDS: Eigenfunction, Numerical Method, T-transform, Padé Approximation

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1. INTRODUCTION

The stationary Schrödinger equation[1] describes the properties of many quantum systems interesting from practical point of view. The eigenvalues and eigenfunctions of this equation cannot be presented in general via analytical expressions for arbitrary

potentials and boundary conditions. For this reason, the equation has to be solved numerically. Two basic general methods have been used in this connection: finite difference method and Fourier transform (mostly in case of periodic potential). The first method cannot obtain precisely the shape of the higher eigenfunctions and needs big computer memory. The second one produces divergent solutions in many cases too. Both methods cannot process effectively the cases of nearly distributed eigenvalues and stiff eigenfunction problems (related to localization phenomena).

The development of a way for general semi-analytical solution of the problem (known as Sturm-Liouville problem) on the basis of non-standard usage of known methods and theoretical results is the subject of the present work.

2. BASIC THEORETICAL RELATIONS

Let us consider the Schrödinger operator in the following equivalent mathematical form [2,3]

$$-\frac{\partial^2 \psi_i(x)}{\partial x^2} + v(x)\psi_i(x) = E_i \psi_i(x), \; i = 0, 1, \ldots, \tag{2.1}$$

where i is an index for the corresponding eigenvalue E_i ($E_i < E_{i+1}$). The lowest eigenvalue is E_0. The index also shows how many times the eigenfunction (bound sate, related to the corresponding eigenvalue) crosses the zero line in its integration interval. [2–3]

In practice, the eigenfunctions $\psi_i(x)$ are normalized in an interval $x \in (x_{min}, x_{max})$ instead of infinity

$$\int_{x_{min}}^{x_{max}} \psi_i^2(x)dx = 1, \qquad i = 0, 1 \ldots$$

(2.2)

Usually, the boundary conditions for the eigenfunction $\psi_i(x)$ are known at the points x_{min} and x_{max}

$$\psi_i(x = x_{min}) = \begin{cases} const., & \text{for the case of periodic wave function} \\ 0, & \text{when } V(x = x_{min}) = V(x = x_{max}) = \infty \end{cases}$$

(2.3)

or for its first derivative

$$\left.\frac{\partial \psi_i(x)}{\partial x}\right|_{x=x_{min}} = \left.\frac{\partial \psi_i(x)}{\partial x}\right|_{x=x_{max}} =$$

$$\begin{cases} const., & \text{for the case of periodic wave function} \\ 0, & \text{when the eigenfunction } \psi \text{ has extremum} \end{cases}$$

(2.4)

representing a two-point boundary Dirichlet problem.

The solution of the equation using the finite difference method needs a high floating point precision and large discrete mesh of points.

Furthermore, the points $x_i^{critical}$ where the eigenvalues E_i cross the potential function $v(x)$ (representing tunneling effect under the existing potential barrier)

$$E_i - v(x = x_i^{critical}) = 0, \qquad i = 0, 1 \ldots$$

(2.5)

are critical for the eigenfunction calculation process [4,5] and the solution becomes divergent, especially for a potential function with complicated form when the eigenvalue crosses the potential barriers many times. But at present this situation is regular considering electronic properties of super-lattices and quantum wells in condensed matter physics.

3. DIFFERENTIAL T-TRANSFORM

Approximately twenty years ago, a new transformation technique named T (Taylor)-transform has been developed by G.E. Poukhov[6,7] in contrast to the well known integral Laplace transforms and Fourier transforms. The T-transform deals with function transforms where the representations are determined by means of the differential operations. Numerous examples from electrical engineering, electronics, mechanics, chemical engineering, heat engineering and computing engineering can be solved using this transform.[6–10]

Supposing the convergency of the corresponding Taylor series for the function $y(x)$ in the interval $x_0 \pm H$, the T-transform consists of the following relations for the image

$$Y(k) = \frac{H^k}{k!} \frac{\partial^k y(x)}{\partial x^k}\bigg|_{x=x_0}, \qquad k = 0, 1, \ldots$$

(3.1)

and the original

$$y(x) = \sum_{k=0}^{\infty} \frac{(x-x_0)^k}{H^k} Y(k)$$

(3.2)

These expressions are known also as DT-$\frac{H^k}{k!}$ - transform.[7]

The basic arithmetic operations for the originals correspond to the following operations for the images

Table 3.1 Basic arithmetic operations for both originals and T-transform images.

ORIGINAL	IMAGE
$y_1(x) + y_2(x)$	$Y_1(k) + Y_2(k)$
$\frac{\partial y(x)}{\partial x}$	$Y(k) = \frac{k+1}{H} Y(k+1)$
$y_1(x)\, y_2(x)$	$Y_1(k)*Y_2(k) = \sum_{l=0}^{k} Y_1(l)Y_2(k-l)$

Note: Here " * " denotes discrete convolution.

Using T-transform, the corresponding image presentation of the Schrödinger equation becomes

$$-\frac{(k+1)(k+2)}{H^2}\,\Psi(k+2) + \sum_{l=0}^{k} \Psi(l)V(k-l) = E_i\,\Psi(k), \qquad k = 0, 1, \ldots \tag{3.3}$$

It is well known that the Taylor series are convergent near to the point x_0 and divergent elsewhere. The T-transform forms a polynomial approximation of k^{th} order to the searching solution near to the point x_0. For this reason, until now the method is used mostly in private cases when the polynomial approximation can successfully describe the searching solution in the integration interval H.

4. ε-ALGORITHM

The convergency of the Taylor series can be improved using corresponding acceleration techniques. The theory of the Padé approximation[10]

$$P(m/n) = \frac{a_0 + a_1 x^1 + \ldots + a_m x^m}{b_0 + b_1 x^1 + \ldots + b_n x^n}$$

(4.1)

as a method for acceleration of Taylor (and non-Taylor) series can be used in the case of T-transform to expand the interval where the initial series can be applied.

One private case of this approach is the ε-algorithm, developed by Shanks[11] and Wynn[12]. The method consists of ε-table construction

Table 4.1 ε-table.

ε_{-1}^{0}	ε_{0}^{0}	ε_{1}^{0}	ε_{2}^{0}	$\cdots$
ε_{-1}^{1}	ε_{0}^{1}	ε_{1}^{1}	$\cdots$	
ε_{-1}^{2}	ε_{0}^{2}	$\cdots$		
ε_{-1}^{3}	$\cdots$			
$\cdots$				

by the following recurrent dependence

$$\varepsilon_{k+1}^{j} = \varepsilon_{k-1}^{j+1} + \frac{1}{\varepsilon_{k}^{j+1} - \varepsilon_{k}^{j}} \qquad (4.2)$$

where $\varepsilon_{-1}^{j} = 0$ and ε_{0}^{j} is the j^{th} sub-sum of the initial series. The column ε_{2}^{j} is identical with the Aitken's acceleration series[10] and only the even columns ($k = 2, 4, 6, \ldots$) give approximation to the searching solution. It can be shown[10] that the ε-table and the Padé approximation table are connected via relation

$$\varepsilon_{2k}^{j} = \mathrm{P}(k+j / k)$$

(4.3)

which explains the convergent properties of the ε-algorithm in cases of Taylor series. The calculation process stops when

$$\varepsilon_k^{j+1} - \varepsilon_k^j = 0$$

(4.4)

i.e., when the necessary floating point precision for the concrete computer variables is reached.[13] In practice, if this condition cannot be satisfied when $k < 100$, this is an indication for the bad convergency of the series and they became divergent.

5. DESCRIPTION OF THE METHOD

In our case, the initial series ε_0^j are the sub-sums of the T-transform series in Eq. (3.2). We note that the ε-algorithm is divergent too far away from the initial point x_0.

The initial T-transform series ε_0^j can be determined if we dispose of information about:

- the eigenvalue E_i;
- the eigenfunction $\psi_i(x = x_0) = \Psi(0)$;
- the eigenfunction's first derivative $\left.\frac{\partial \psi_i(x)}{\partial x}\right|_{x=x_0} = \Psi(1)$.

Here E_i is unknown. At arbitrary E-value, starting from the boundary point $x_0 = x_{min}$, where

- $\Psi(0) = 0$ (eigenfunction zero point), supposing $\Psi(1) = const.$

or

- $\Psi(1) = 0$ (eigenfunction extremum point), supposing $\Psi(0) = const.$

the ε-algorithm can be applied toward the series (3.2) to obtain a corresponding point x_{new} ($x_{min} < x_{new} \leq x_{max}$) where the ε-algorithm is still convergent for the T-transform series. Then we can determine new series (3.2) for the new point $x_0 = x_{new}$. It is convenient to set x_{new} at a point where the eigenfunction has extremum ($\Psi(1) = 0$) or crosses the zero line ($\Psi(0) = 0$). This extremum or zero point can be determined using binary search method. The aforesaid procedure can continue until x_{max} is reached.

For two different values E_i^{min} and E_i^{max} one can obtain two different solutions $\psi_i(E_i^{min}, x)$ and $\psi_i(E_i^{max}, x)$, $x = (x_{min}, x_{max})$, which have corresponding values at the point x_{max}: $\psi_i(E_i^{min}, x = x_{max})$ and $\psi_i(E_i^{max}, x = x_{max})$. This approach is well known in the literature as shooting method.[4] The second boundary condition can be reached using binary search method

$$E_i^{new} = (E_i^{max} + E_i^{min}) / 2 \qquad (5.1)$$

E_i^{new} corresponds to a new limit E_i^{max} or E_i^{min}. It is well known that the eigenfunction $\psi_i(x)$ crosses i times the zero point in the integration interval (x_{min}, x_{max}).[4] Let $i_{crossing}$ denotes how many times $\psi_i(E_i^{new}, x)$ crosses the zero point in the integration interval. If $i_{crossing} < i$, then $E_i^{min} = E_i^{new}$, else $E_i^{max} = E_i^{new}$. The shooting process continues until the needed precision for the eigenvalues E_i is obtained.

Our method allows one to obtain precisely each consecutive point of the eigenfunction (including the second boundary point $\psi_i\ (x = x_{max})$ during the shooting process. For this reason, the determination of the eigenvalues is so effective in contrast to the shooting process applies in combination with the finite difference method.[4]

The presented method has the following advantages in comparison with the other methods :

- precise determination of nearly distributed eigenvalues;
- precise determination of higher eigenfunctions, especially at its extremum and zero points;
- there is no need to solve systems of linear equations as in the case of finite difference method or Fourier transform method;
- the numerical quick-action increases, since the ε-algorithm ensures large steps passing the integration interval;
- the needed computer memory for the numerical algorithm is very small;
- stiff eigenfunction problems can be solved, since the step in the integration interval decreases or increases depending on the acceleration properties of the ε-algorithm.

6. APPLICATION TO MATHIEU'S FUNCTION

In this section we will show the power of the presented method solving a difficult problem of the mathematical physics, where the existing at present methods do not work properly.

The Mathieu function[14,15] (elliptic cylinder function) as a solution of the Sturm-Liouville problem of the equation

$$-\frac{\partial^2 \psi_i(x)}{\partial x^2} + 2q\cos(2x)\,\psi_i(x) = E_i\,\psi_i(x), \qquad i = 0, 1, \ldots$$

(6.1)

represents a special function with period 2π. Here $v(x)= 2q\cos(2x)$. The default normalization of this function in the literature is

$$\int_0^{2\pi} \psi_i^2(x,q)dx = \pi$$

(6.2)

The function describes an one-dimensional rotator in cosinusoidal potential with height $2q$. The localization of the rotator rises increasing q. The values up to $q = 20$ are interesting from practical point of view.

The analytical solutions of the Mathieu function using Fourier transform are well known.[14,15] In universally accepted designations the following functions correspond to the eigenvalues E_i as follows:

for $i = 4n$, $n = 0, 1, \ldots$ (even functions with period π):

$$\mathrm{ce}_{2m}(x, q) = \sum_{k=0}^{\infty} A_{2m,2k}\cos(2kx), \qquad m = 0, 1, \ldots$$

(6.3)

for $i = 4n + 1$, $n = 0, 1, \ldots$ (odd functions with period 2π):

$$\mathrm{se}_{2m+1}(x, q) = \sum_{k=0}^{\infty} B_{2m+1,2k+1}\sin[(2k+1)x], \qquad m = 0, 1, \ldots$$

(6.4)

for $i = 4n + 2$, $n = 0, 1, \ldots$ (even functions with period 2π):

$$\mathrm{ce}_{2m+1}(x, q) = \sum_{k=0}^{\infty} A_{2m+1,2k+1}\cos[(2k+1)x], \qquad m = 0, 1, \ldots$$

(6.5)

for $i = 4n + 3$, $n = 0, 1, \ldots$ (odd functions with period π):

$$\mathrm{se}_{2m}(x, q) = \sum_{k=1}^{\infty} B_{2m,2k}\sin(2kx), \qquad m = 1, 2, \ldots$$

(6.6)

The eigenvalues E and the coefficients A and B can be found from the basic recurrent dependence

$$qC_{s,r-2} + (E - s^2)C_{s,r} + qC_{s,r+2} = 0,\ C = A,\ B;\ s = 2m,\ 2m+1;\ r = 2k,\ 2k+1 \quad (6.7)$$

The initial dependencies for the different functions are:

for $ce_{2m}(x, q)$: $2qA_{2m,0} + (E - 4^2)A_{2m,2} + qA_{2m,4} = 0;\ EA_{2m,0} + qA_{2m,2} = 0$

(6.8)

for $ce_{2m+1}(x, q)$: $(E - 1 + q)A_{2m+1,1} + qA_{2m+1,3} = 0$

(6.9)

for $se_{2m+1}(x, q)$: $(E - 1 - q)B_{2m+1,1} + qB_{2m+1,3} = 0$

(6.10)

for $se_{2m}(x, q)$: $(E-4)B_{2m,2} + qB_{2m,4} = 0$

(6.11)

These dependencies form infinite three-diagonal matrices. For example, the three-diagonal determinant of the matrix for $ce_{2m}(x, q)$ has the form

$$\begin{Vmatrix} E & q & 0 & 0 & \dots \\ 2q & E-4 & q & 0 & \dots \\ 0 & q & E-16 & q & \dots \\ 0 & 0 & q & E-36 & \dots \\ \dots & \dots & \dots & \dots & \dots \end{Vmatrix} = 0$$

(6.12)

The first *30* eigenvalues can be obtained from Eq. (6.12) with more than *16* true digits using no more than *200* initial elements of the infinite matrix. The asymmetry of the first sub-diagonal elements (q and $2q$) can be removed since the initial determinant is

equivalent to a symmetric determinant with first sub-diagonal elements equal to $\sqrt{2}\,q$. The eigenvalues can easily be found with the needed precision using the well developed iterative methods for these infinite matrixes. The most powerful method for obtaining the eigenvalues of symmetric three-diagonal matrix consists of the extension of the corresponding determinant in Sturm series. A very fast and effective algorithm (especially for nearly distributed eigenvalues) has been realized in the procedure BISECT.[16]

However, the eigen functions cannot be obtained from the Fourier series (6.3-6.6) since they are divergent at $q > 1$. The acceleration properties of the ε-algorithm applied toward these series do not work properly. The numerical solution for the higher eigenfunctions using finite difference method is also not effective at $q > 1$.

Using the method presented in this paper, we can obtain a solution at extremely high $q=100$ (which corresponds to non-physical strong localization) and can determine, for example, the initial *30* eigenvalues and eigenfunctions.[17]

Fig.1 represents the dependence $E_i(q)$, q = *-100 . . . 100*. The form of the potential and corresponding eigenvalues at $q=100$ are shown in Fig.2. In this figure the initial even and odd eigenvalues with different period (π and 2π) in practice coincide with more than *6* true digits.

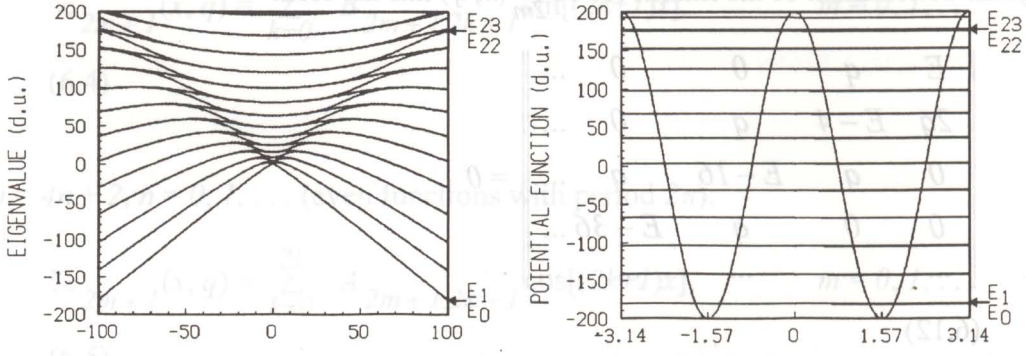


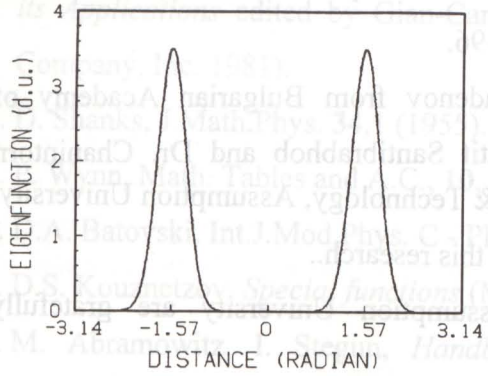
Figure 1. Eigenvalues of Mathieu's equation as a function of the q-parameter (on the left).

Figure 2. Potential function and eigenvalues ($q=100$) (on the right).

Starting from $x_0 = 0$ one can obtain the eigenfunctions in the interval $[-\pi/2, \pi/2]$ without any change of x_0. After that one can choose new points $x_0 = -\pi$ and $x_0 = \pi$ to obtain the eigenfunctions in the intervals $[-\pi, -\pi/2]$ and $[\pi/2, \pi]$.

The normalized eigenfunction $\psi_0(x) = \mathrm{ce}_0(x)$ at $q=100$ is presented in Fig.3. It can be seen that the higher localization of the eigenfunction corresponds to a stiff numerical problem.

The normalized eigenfunction $\psi_{23}(x) = \mathrm{se}_{12}(x)$ at $q=100$ is shown in Fig.4. The eigenfunction crosses *23* times the zero point. The finite difference method will need very fine mesh of discrete points and higher numerical precision to obtain the shape presented in the figure.



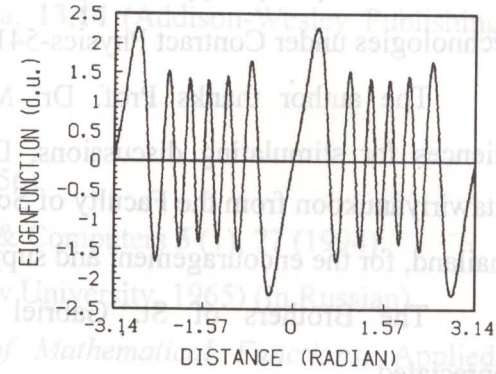


Figure 3. Eigenfunction $\psi_0(x)$ $(q=100)$ (on the left).

Figure 4. Eigenfunction $\psi_{23}(x)$ $(q=100)$ (on the right).

In practice, our method can find precisely the eigenfunctions only, if the eigenvalues can be obtained easily using some different method as in the case of Mathieu's function. However, the shooting method is very effective for solving the problem in general.

7. CONCLUSION

In this paper we have presented an ultimate method for semi-analytical solution in general of the stationary Schrödinger equation. The differential T-transform in connection with ε-table acceleration can be used in many related problems of the mathematical physics.

The extension of the method for solving two- and three-dimensional Schrödinger equations on the basis of two- and three- dimensional T-transforms[7] is based on the same idea. The theoretical and numerical treatment of many-dimensional T-transform acceleration techniques will be published in an additional paper.

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