Численные методы и их приложения

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Numerical Solutions for the Schrödinger Equation with a Degenerate Polynomial Potential of Even Power

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A high order finite difference scheme for the Schrödinger equation with the degenerate potential $U(x) = x^{2r}$, $r \in N$, which describes phase transitions in quantum systems, have been constructed. The eigenvalues are found for some values of r.

Key words and phrases: Schrödinger equation, finite difference scheme, shooting method, eigenvalue, optimal spline.

1. Introduction

We consider the one-dimensional Schrödinger equation

$$u'' + (\lambda - q(x))u = 0, \tag{1}$$

with the limiting conditions for eigenstates $\int\limits_{-\infty}^{+\infty} u^2(x)\mathrm{d}x < \infty$. The aim of this paper is the calculation of the eigenvalues λ_n $(n = 0, 1, \ldots)$ of the equation (1) when the potential function $q(x)$ is of the type:

$$q(x) = x^{2r}, \quad r = 1, 2, \ldots \ .$$

From the practical viewpoint, it is especially interesting to solve the Schrödinger equation with this potential. The reasons for the interest in the potential of this form are the following. First, in many cases, the relativistic Dirac and Klein-Gordon-Fock equations can be presented in such a form after separating the variables. The second reason is more significant from the viewpoint of physical applications. Potentials of the form x^{2r} correspond to the critical situation where all coefficients in the polynomial $P_{2r}(x)$, except the highest one, turn to zero. This situation implies degeneracy and is usually considered when studying phase transitions in critical systems [1].

2. The Higher Order Method

We rewrite the equation (1) in the form

$$\begin{gathered} u'' = -f(x)u, \\ u(x) \to 0, \quad x \to \pm\infty, \end{gathered} \tag{2}$$

where $f(x) = \lambda - q(x)$.

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We will construct a $2m \quad (m \geqslant 1)$ order method for the equation (2). If differentiating the equation (2), we can find that

$$\begin{gathered} u^{(2k-1)} = (-f)^{k-1}u' + A_{2k-1}u + B_{2k-1}u', \quad k \geqslant 2, \\ u^{(2k)} = (-f)^k u + A_{2k}u + B_{2k}u', \end{gathered} \tag{3}$$

where coefficients A_n and B_n are depends from $f(x)$ and it's derivatives. In (4) we are present the coefficients A_n and B_n from $n = 3$ through 8.

$$\begin{gathered} A_3 = -f', \quad B_3 = 0, \\ A_4 = -f'', \quad B_4 = -2f', \\ A_5 = 4ff' - f''', \quad B_5 = -3f'', \\ A_6 = 7ff'' + 4f'^2 - f^{IV}, \quad B_6 = 6ff' - 4f''', \\ A_7 = -9f^2f' + 11ff''' + 15f'f'' - f^V, \quad B_7 = 13ff'' + 10f'^2 - 5f^{IV}, \\ A_8 = -22f^2f'' - 28ff'^2 + 16ff^{IV} + 26f'f''' + 15f''^2 - f^{VI}, \\ B_8 = -12f^2f' + 24ff''' + 48f'f'' - 6f^V. \end{gathered} \tag{4}$$

Using Taylor expansion and (3), we obtain

$$\begin{gathered} u_{i+1} + u_{i-1} = 2a_1u_i + 2b_1u_i' + O(h^{2m+2}), \\ u_{i+1} - u_{i-1} = 2a_2u_i + 2b_2u_i' + O(h^{2m-1}), \end{gathered} \tag{5}$$

where,

$$\begin{gathered} a_1 = \mathrm{cs}(f_i, h) + \sum_{k=2}^{m} A_{2k}\frac{h^{2k}}{(2k)!}, \quad b_1 = \sum_{k=2}^{m} B_{2k}\frac{h^{2k}}{(2k)!}, \\ a_2 = \sum_{k=2}^{m-1} A_{2k-1}\frac{h^{2k-1}}{(2k-1)!}, \quad b_2 = \mathrm{sn}(f_i, h) + \sum_{k=2}^{m-1} B_{2k-1}\frac{h^{2k-1}}{(2k-1)!}, \\ \mathrm{cs}(f,h) = \begin{cases} \cos\sqrt{f}h, & f \geqslant 0, \\ \cosh\sqrt{|f|}h, & f < 0, \end{cases} \quad \mathrm{sn}(f,h) = \begin{cases} \dfrac{\sin\sqrt{f}h}{\sqrt{f}}, & f > 0, \\ h, & f = 0, \\ \dfrac{\sinh\sqrt{|f|}h}{\sqrt{|f|}}, & f < 0. \end{cases} \end{gathered} \tag{6}$$

If to eliminate u_i' from (5), then we obtain $2m$-th order integration formula

$$\begin{gathered} (b_2 - b_1)u_{i+1} - 2(a_1b_2 - a_2b_1)u_i + (b_2 + b_1)u_{i-1} = 0, \\ u_0 = u_N = 0, \quad i = 1, \dots, N-1. \end{gathered}$$

The main disadvantage of the method is that we have used the derivatives of the potential function $q(x)$. If the potential function is more complicated, we can approximate derivatives of the potential without decreasing the order of the method. For example, if $m = 4$, we will use optimal cubic spline [2].

Def. The cubic spline interpolation $S(x)$, with boundary conditions

$$82M_0 + 339M_1 = -5f_0'' + \frac{6381f_{\overline{x}x,1} - 1522f_{\overline{x}x,2} + 281f_{\overline{x}x,3} - 28f_{\overline{x}x,4}}{12},$$

$$339M_{N-1}+82M_N=-5f''_N+\frac{6381f_{\overline{x}x,N-1}-1522f_{\overline{x}x,N-2}}{12}+$$
$$+\frac{281f_{\overline{x}x,N-3}-28f_{\overline{x}x,N-4}}{12},$$

are called optimal cubic spline for $f(x)$, where $M_i=S''(x_i)$, $\quad m_i=S'(x_i)$,

Theorem 1. *Let S be an optimal cubic spline interpolation for $f(x)$. Then*

$$f'_i=m_i+\frac{\delta^4 m_i}{180}+O(h^6),\quad i=0(1)N,$$

$$f''_i=M_i+\frac{\delta^2 M_i}{12}-\frac{\delta^4 M_i}{360}+O(h^6),\quad i=1(1)N-1,$$

$$f''_0=M_0+\frac{\delta^2 M_0}{12}+\frac{57\delta^4 M_2-28\delta^4 M_3}{360}+O(h^6),$$

$$f''_N=M_N+\frac{\delta^2 M_N}{12}+\frac{57\delta^4 M_{N-2}-28\delta^4 M_{N-3}}{360}+O(h^6),$$

$$f'''_i=m_{\overline{x}x,i}-\frac{\delta^4 m_i}{12h^2}+O(h^4),\quad i=1(1)N-1,$$

$$f'''_0=m_{\overline{x}x,0}+\frac{10\delta^4 m_1+\delta^4 m_2}{12h^2}+O(h^4),$$

$$f'''_N=m_{\overline{x}x,N}+\frac{10\delta^4 m_{N-1}+\delta^4 m_{N-2}}{12h^2}+O(h^4),$$

$$f^{IV}_i=M_{\overline{x}x,i}+O(h^4),\quad i=1(1)N-1,$$

$$f^{IV}_0=M_{\overline{x}x,0}+\frac{\delta^4 M_1}{h^2}+O(h^4),\quad f^{IV}_N=M_{\overline{x}x,N}+\frac{\delta^4 M_{N-1}}{h^2}+O(h^4),$$

$$f^{V}_i=\frac{\delta^4 m_i}{h^4}+O(h^2),\quad i=0(1)N,\quad f^{VI}_i=\frac{\delta^4 M_i}{h^4}+O(h^2),\quad i=0(1)N,$$

where the difference operators $\delta^2 f_i$ and $\delta^4 f_i$ are defined by

$$\delta^2 f_i=f_{i+1}-2f_i+f_{i-1},\quad i=1(1)N-1,$$

$$\delta^2 f_0=2\delta^2 f_1-\delta^2 f_2,\quad \delta^2 f_N=2\delta^2 f_{N-1}-\delta^2 f_{N-2},$$

$$\delta^4 f_i=f_{i+2}-4f_{i+1}+6f_i-4f_{i-1}+f_{i-2},\quad i=2(1)N-2,$$

$$\delta^4 f_0=3\delta^4 f_2-2\delta^4 f_3,\quad \delta^4 f_1=2\delta^4 f_2-\delta^4 f_3,$$

$$\delta^4 f_N=3\delta^4 f_{N-2}-2\delta^4 f_{N-3},\quad \delta^4 f_{N-1}=2\delta^4 f_{N-2}-\delta^4 f_{N-3},\quad f_{\overline{x}x,i}=\frac{\delta^2 f_i}{h^2}.$$

3. Numerical Results

For the purpose of numerical computation, we take the domain of integration to be $[-L,L]$. The value of L depends from r and decreasing, while the power r increasing.

r	2	3	4	5	6	7
L	4.17	3.65	2.50	2.25	2.11	1.89

Table 1

First 30 calculated eigenvalues

n	r=2	r=3	r=4	r=5	r=6	r=7
0	1.0603620904	1.1448024537	1.2258201138	1.2988437006	1.3637614851	1.4214388844
1	3.7996730298	4.3385987115	4.7558744139	5.0978765292	5.3869415656	5.6361850305
2	7.4556979379	9.0730845609	10.2449469772	11.1543182021	11.8930091123	12.5121019946
3	11.6447455113	14.9351696349	17.3430879705	19.1888095590	20.6616375799	21.8747752044
4	16.2618260188	21.7141654221	25.8090067512	28.9714672126	31.4894713768	33.5498907390
5	21.2383729182	29.2996459374	35.4978988051	40.3426154415	44.2180537634	47.3892749833
6	26.5284711836	37.6130865608	46.3127704950	53.1923057711	58.7311562516	63.2767962314
7	32.0985977109	46.5952114485	58.1796499496	67.4382131585	74.9412167421	81.1225070124
8	37.9230010270	56.1993008524	71.0392576758	83.0142870755	92.7784725989	100.8546171552
9	43.9811580972	66.3872817065	84.8426245922	99.8655565423	112.1848895673	122.4135995997
10	50.2562545166	77.1273414638	99.5483528576	117.9451915673	133.1108600535	145.7486045046
11	56.7342140551	88.3923757690	115.1208011087	137.2125942515	155.5131898491	170.8152866328
12	63.4030469867	100.1589278926	131.5288311156	157.6320739504	179.3537421724	197.5743944699
13	70.2523946286	112.4064358114	148.7449100322	179.1718917958	204.5984667291	225.9907866168
14	77.2732004819	125.1166807475	166.7444474448	201.8035511287	231.2166778832	256.0327095224
15	84.4574662749	138.2733726559	185.5052932361	225.5012574295	259.1805036463	287.6712481759
16	91.7980668089	151.8618317586	205.0073490402	250.2414985330	288.4644561000	320.8798978399
17	99.2886066604	165.8687392469	225.2322620498	276.0027124124	319.0450904591	355.6342237056
18	106.9233073817	180.2819389410	246.1631798748	302.7650201269	350.9007302761	391.9115861187
19	114.6969173849	195.0902772336	267.7845515500	330.5100082148	384.0112429461	429.6909157169
20	122.6046390010	210.2834723147	290.0819640251	359.2205492343	418.3578541100	468.9525272161
21	130.6420687486	225.8520060937	313.0420063488	388.8806521792	453.9229925879	509.6779635721
22	138.8051479113	241.7870340565	336.6521554770	419.4753366044	490.6901595936	551.8498643340
23	147.0901212576	258.0803093041	360.9006813579	450.9905257883	528.6438174875	595.4518534902
24	155.4935022687	274.7241181146	385.7765605338	483.4129553541	567.7692944210	640.4684431920
25	164.0120436230	291.7112248219	411.2694154301	516.7300945457	608.0527020321	686.8849505305
26	172.6427119633	309.0348243637	437.3694321200	550.9300779992	649.4808639504	734.6874251454
27	181.3826661875	326.6885011755	464.0673526269	586.0016461959	692.0412533314	783.8625858836
28	190.2292386581	344.6661988392	491.3543345388	621.9340933429	735.7219379842	834.3977650941
29	199.1799188370	362.9621614217	519.2221047363	658.7172212546	780.5115319321	886.2808593737

To calculate the eigenvalues, we have used 8 order formula ($m = 4$) and shooting method. We need to know the value of u_1.

Taking advantage of the fact that the problem has explicit symmetry with respect to the transformation $x \mapsto -x$, we first seek all even solutions of Eq.(1) that satisfy

$$u(0) = 1, \quad u'(0) = 0.$$

We can calculate u_1 by using the formula

$$u_1 = \mathrm{cs}(\lambda, h) + \sum_{k=r+1}^{m} A_{2k} \frac{h^{2k}}{(2k)!}.$$

For the odd solutions satisfying the conditions

$$u(0) = 0, \quad u'(0) = 1,$$

we have calculated u_1 by the formula

$$u_1 = \mathrm{sn}(\lambda, h) + \sum_{k=r+2}^{m} B_{2k-1} \frac{h^{2k-1}}{(2k-1)!}.$$

Table 1 shows first 30 calculated eigenvalues. The results coincide with [3].

References

1. *Vshivzev A. S., Norin N. V., N.Sorokin V.* Solution of the Spectral Problem for the Schrödinger Equation with a Degenerate Polynomial Potential of Even Power // Theor. Math. Phys. — 1996. — Vol. 109, No 1. — Pp. 107–123.
2. *Zhanlav T.* On a Optimal Cubic Spline and its Application to Numerical Analysis // Scientific Transactions. — 1998. — Vol. 1.
3. *Hautot A., Magnus A.* Calculation of the Eigenvalues of Schrödinger Equations by an Extension of Hill's Method // J. Comp. Appl. Math. — 1979. — Vol. 5, No 1. — Pp. 3–15.

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Численные решения для уравнения Шрёдингера с вырожденным полиномным потенциалом чётной степени

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Построена конечно-разностная схема высокого порядка для уравнения Шрёдингера с вырожденным потенциалом $U(x) = x^{2r},\ r \in N$, которая описывает фазовые переходы в квантовых системах. Для некоторых значений r найдены собственные значения.

Ключевые слова: уравнение Шрёдингера, конечно-разностная схема, собственные значения, метод стрельбы, оптимальный сплайн.