

Solution of Certain Potential Problems by the Asymptotic Iteration Method and Verification of the Results by Matlab Code.

Abhijit Sidhanta

Bankim Sardar College Canning, 24 Parganas (South)

West Bengal, India

Email – abhijit.sidhanta@gmail.com

Abstract: We apply the asymptotic iteration method (AIM) to solve for the eigenvalues of the Gol'dman Krivchenko potential and quatriconharmonic potential and verify the results using Matlab codes.

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I. Introduction:

Second order homogeneous linear differential equations occur in many fields of mathematical physics. In literature mention is made of many techniques to solve them viz. supersymmetry (SUSY) [1], the Nikiforov-Uvarov method [2], the Pekeris approximation [3], asymptotic iteration method (AIM) [4]. We shall however take recourse to the asymptotic iteration method to solve second order homogeneous linear differential equations of the Schrodinger type though other equations can as well be solved by this technique. Our work is divided into five sections. Section 2 gives a brief introduction to the asymptotic iteration method. Section 3 deals with the underlying numerical analysis part – finite difference method to solve for the eigenvalues of the Schrodinger equation employed in our Matlab solution for the eigenvalues of the Schrodinger equation. Section 4 consists of solving for the eigenvalues of the Schrodinger equation with a) Gol'dman Krivchenko potential [5] b) quatriconharmonic potential along with the Matlab codes to solve for the eigenvalues of the Schrodinger equation based on the aforesaid finite difference method. In Section 5 we draw the conclusion from our work.

II. Asymptotic Iteration Method:

The solution of the Schrodinger equation by the asymptotic iteration method consists of two parts viz. i) finding the eigenvalues of the problem and ii) finding the wavefunctions. In our case we will discuss only the case of finding the eigenvalues of the problem since finding the wavefunctions is not our goal here though it can be done quite easily.

Consider the second order homogeneous linear differential equation,

$$y'' = \lambda_0(x)y' + s_0(x)y \quad (1)$$

where $\lambda_0(x)$ and $s_0(x)$ are functions in $C_\infty(a, b)$. This has a solution if for some

$$n > 0, \frac{s_n}{\lambda_n} = \frac{s_{n-1}}{\lambda_{n-1}} = \alpha \quad (2)$$

$$\text{where } \lambda_k = \lambda'_{k-1} + s_{k-1} + \lambda_0 \lambda_{k-1} \text{ and } s_k = s'_{k-1} + s_0 \lambda_{k-1} \quad (3)$$

for $k=1, 2, 3, \dots, n$.

We however do not go into the solution of (1) for y . One can look up [4]. As claimed before our task is to find the eigenvalues for the two cases we consider and verify the eigenvalues by a use of the Matlab codes we present.

III. Numerical Solution Using Finite Difference Matrix Method

In natural units the Schrodinger equation reads

$$-\frac{1}{2} \frac{d^2 \psi}{dx^2} + V(x)\psi = E\psi \quad (4)$$

Using the finite difference approximation this can be written as

$$-\frac{1}{2} \frac{\psi_{i+1} - 2\psi_i + \psi_{i-1}}{(\Delta x)^2} + V_i \psi_i \approx E\psi_i$$

$$\left(\frac{1}{(\Delta x)^2} - V_i - E \right) \psi_i - \frac{1}{2(\Delta x)^2} \psi_{i-1} - \frac{1}{2(\Delta x)^2} \psi_{i+1} = 0 \quad (5)$$

In the matrix form,

$$\begin{pmatrix} \frac{1}{(\Delta x)^2} - V_2 - E & -\frac{1}{2(\Delta x)^2} & 0 & 0 \\ -\frac{1}{2(\Delta x)^2} & \frac{1}{(\Delta x)^2} - V_3 - E & -\frac{1}{2(\Delta x)^2} & 0 \\ 0 & -\frac{1}{2(\Delta x)^2} & \frac{1}{(\Delta x)^2} - V_4 - E & -\frac{1}{2(\Delta x)^2} \\ 0 & 0 & -\frac{1}{2(\Delta x)^2} & \frac{1}{(\Delta x)^2} - V_5 - E \end{pmatrix} \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \end{pmatrix} \quad (6)$$

IV. Analytical and Matlab solution of the eigenvalues by AIM:

4.1 Gol'dman and Krivchenko potential:

The Gol'dman and Krivchenko potential is a generalization of the 3-dimensional harmonic oscillator. The Schrodinger equation in this case takes the form

$\frac{1}{2} \left(-\frac{d^2}{dr^2} + r^2 + \frac{\gamma(\gamma+1)}{r^2} \right) \psi = E\psi$ (7), in natural units, where $\psi = L_2(0, \infty)$ and satisfies the condition $\psi = 0$ as the Dirichlet boundary condition. The generalization stems from the parameter γ ranging over $(0, \infty)$ instead of the angular momentum quantum number $l=0,1,2,\dots$. For large r , the solution of (4) behaves like the exact solutions of the harmonic oscillator. Hence it is reasonable to assume the unnormalised ψ as

$$\psi(r) = r^{\gamma+1} e^{-r^2/2} f(r) \quad (8)$$

where $f(r)$ can be determined from the above mentioned iteration procedure. Substituting (5) in (4) we get,

$$\frac{d^2 f}{dr^2} = 2 \left(r - \frac{\gamma+1}{r} \right) \frac{df}{dr} + [2\gamma + 3 - 2E]f = 0 \quad (9).$$

This equation is however slightly different from its counterpart in eqn. (3.13) in [4]. This is because in eqn (4) we have taken the exact Hamiltonian of the Harmonic oscillator whereas in eqn. (3.11) of [4] the authors have taken a slightly modified Hamiltonian.

$$\text{In our case } \lambda_0(r) = 2 \left(r - \frac{\gamma+1}{r} \right) \text{ and } s_0(r) = 2\gamma + 3 - 2E \quad (10).$$

The AIM condition (2) has to be satisfied here. Here $\frac{s_0}{\lambda_0} = \frac{2\gamma+3-2E}{2 \left(r - \frac{\gamma+1}{r} \right)}$ (11.1)

$$\frac{s_1}{\lambda_1} = \frac{(2\gamma+3-2E)4 \left(r - \frac{\gamma+1}{r} \right)}{2\gamma+3-2E+2 \left(1 + \frac{\gamma+1}{r^2} \right) + 4 \left(r - \frac{\gamma+1}{r} \right)^2} \quad (11.2)$$

Since here $\lambda_{n+1}s_n - s_{n+1}\lambda_n$ depend on r and is not a constant we have to force certain conditions on (8.1) and (8.2). We start by setting $s_0 = 0$ in (11.1) which give us the first eigenvalue $E_1 = \frac{1}{2}(2\gamma + 3)$ (12). Again putting $s_1 = 0$ in (11.2) we arrive at the result $r^2 = \gamma + 1$ (13) since the other factor in the numerator of the RHS of (11.2) i.e. $2\gamma + 3 - E_2$ cannot be zero because of (12).

Inspecting equations (11.1) and (11.2) we find that for the AIM condition (2) to hold

$$2\gamma + 3 - 2E_2 + 2 \left(1 + \frac{\gamma+1}{r^2} \right) = 0 \quad (14)$$

Using (10) in (11) we immediately obtain the second eigenvalue i.e.

$$E_2 = \frac{1}{2}(2\gamma + 7) \quad (15)$$

In this way we can also find $E_3 = \frac{1}{2}(2\gamma + 11)$ (16)

$$\text{Generalising, } E_n = \frac{1}{2}(2\gamma + 3 + 4n) \quad (17)$$

where $n=0,1,2,3,\dots$. Equation (17) was an outcome of certain ad hoc forcing of conditions. Next we compute the eigenvalues of this problem by Matlab.

Matlab code for determination of the eigenvalues for Goldman Krivchenko potential in 1D

```
V = inline('x*x+(0.5*1.5)*(1.0/(x*x))'); % the potential
n = 2000; % number of parts
xL= 0.001;% left end where psi(xL)=0
xR= 10; % right end where psi(xR)=0
dx= (xR-xL)/n;
x = xL;
A = zeros(n-1); % matrix elements
%B=1.5;
for i=1:n-1
for j=1:n-1
if (i==j+1 || i==j-1)
A(i,j) = -1.0*((1.0)/(dx^2));
```

```

end
end
x = x + dx;
A(i,i) = (2.0)/(dx^2) + V(x);
end

[wfn E] = eig(A); % get eigenvalues and eigenvectors

x = xL+dx:dx:xR-dx;
fprintf('*** Energy eigenvalues for bound states ***\n',n);
for i=1:5
energy(i) = E(i,i);
fprintf('n=%2d --> E=%15.4f\n',i,energy(i));
end

```

Output

```

*** Energy eigenvalues for bound states ***
n= 1 --> E= 2.0000
n= 2 --> E= 4.0000
n= 3 --> E= 5.9999
n= 4 --> E= 7.9999
n= 5 --> E= 9.9998

```

Putting the values of n and $\gamma = 0.5$ in (17) gives values of E_n which agrees with this Matlab result and this in turn vindicates our AIM result. One comment is in order here. The value of E_0 as obtained from (17) agrees with the E_1 result obtained in above by Matlab. This is because Matlab treats any variable as a matrix and the (0,0) element of a matrix does not exist.

4.2 Quatricanharmonic potential

Next we treat the case of anharmonicquartic potential by the AIM. The Schrodinger equation in this case in one dimension is,

$$\left(-\frac{1}{2} \frac{d^2}{dx^2} + \frac{1}{2}x^2 + Ax^4\right)\psi = E\psi \quad (18).$$

The unnormalised ψ is, $\psi(x) = e^{-\frac{x^2}{2}} f(x)$ (19).

Substituting (19) in (18) we obtain,

$$\frac{d^2f}{dx^2} = 2x \frac{df}{dx} + (1 - E + Ax^4)f \dots\dots\dots(20).$$

Using $\lambda_0(x) = 2x$ and $s_0(x) = (1 - E + Ax^4)$ (21)

and the termination condition $\delta = \lambda_{n+1}s_n - \lambda_n s_{n+1}$ (22) we get the solutions for the eigenvalues in two possible ways as before. We first present the Matlab solution and since this problem has no exact solution and derive the eigenvalues by the AIM in harmony with the Matlab eigenvalues.

Matlab code for determination of the eigenvalues for quatricanharmonic potential

```

V = inline('0.5*x*x+0.5*0.1*x*x*x*x'); % the potential
L = 1.0; % width
n = 2000; % number of parts
xL= -10*L; % left end where psi(xL)=0
xR= 10*L; % right end where psi(xR)=0
dx= (xR-xL)/n;
x = xL;
A = zeros(n-1); % matrix elements

for i=1:n-1
for j=1:n-1
if (i==j+1 || i==j-1)
A(i,j) = -1.0/dx^2;
end

```

```

end
x = x + dx;
A(i,i) = 2.0/dx^2 + V(x);
end

[wfn E] = eig(A); % get eigenvalues and eigenvectors

x = xL+dx:dx:xR-dx;
fprintf('*** Energy eigenvalues for bound states ***\n',n);
for i=1:5
energy(i) = E(i,i);
fprintf('n=%2d --> E=%15.4f\n',i,energy(i));
end
Output
*** Energy eigenvalues for bound states ***
n= 1 --> E=    0.5326
n= 2 --> E=    1.6534
n= 3 --> E=    2.8739
n= 4 --> E=    4.1762
n= 5 --> E=    5.5491
    
```

Putting different n , forcing $\delta = 0$ in (22) and using (21) we get by AIM the following values of the eigenvalues for $A=0.1$ as depicted in Table . 1

n	E^A	Corresponding Value of x	E^M
0	0.5326	± 1.2433	1.065286
1	1.6534	± 2.93548	3.306872
2	2.8739	± 3.14410	5.747959
3	4.1762	± 3.31265	8.352678
4	5.5491	± 3.45726	11.09860

Table.1 E^A are the eigenvalues obtained by us whereas E^M are the eigenvalues obtained by direct numerical integration of Schrodinger equation [6]. Due to our choice of the form of the Schrodinger equation E^A is exactly half of E^M .

V. Conclusions

We conclude that asymptotic iteration method is a powerful to solve allsecond order homogeneous linear differential equations. Since these differential equations have widespread applications in Physics the scope of the application of AIM is numerous.

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