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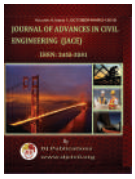

RESEARCH ARTICLE

Solution of the Eigenvalue Problems by using Galerkin Finite Element Method for an External Potential

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ABSTRACT

A numerical solution of the linear Schrödinger Equation (SE) is found using the Galerkin Finite element method. Test problems were greatly concerned with the external potential which form the core of the paper. First the Schrödinger eigenvalue problem is derived and then it is solved by a finite element method numerically. Finally the numerical results of eigen values and eigen vectors are compared with the exact solutions.

Keywords: Linear Schrödinger equation, Galerkin finite element method, External potential, Eigen vectors, Eigen values.

1. INTRODUCTION

As we know that the exact solution of Schrödinger Equation (SE) is not possible in complicated situations it is preferred to apply some numerical techniques such as FDM, FEM etc. in such conditions. In non-relativistic quantum mechanics, one of the basic and fundamental equations is the SE. SE mainly deals with the atomistic or molecular configurations especially the time evolution of a quantum state [1-5]. Now the challenge is to find the SE solution [6-8]. Hydrogen atom has a very "simple" atomistic configuration and analytical solutions are available only for such atoms. Further it is a highly tedious process, numerically to obtain the equation except for particles with less size. The paper starts with a time dependent Schrödinger equation which has a time independent potential. Next the eigenvalue problem is derived and computed. The principal eigenvalue represents the ground state. We choose Galerkin FEM to find the eigenvalues and eigenvectors for one dimensional and two dimensional linear Schrödinger equation with small and large potentials [9]. The analysis is shown in equations [1] to [28].

1.1. The time dependent Schrödinger equation

The time dependent SE is a universal form which gives a system description evolving with time and it is highly essential in stationary state systems.

The SE for a single particle with potential energy U(x) reads,

$$i\hbar\frac{\partial}{\partial t}\psi(x,t)=\left(-\frac{\hbar^2}{2m}\nabla^2+U(x)\right)\psi(x,t)=-\frac{\hbar^2}{2m}\nabla^2\psi(x,t)+U(x)\psi(x,t) \tag{1}$$

where, $-\frac{\hbar^2}{2m}\nabla^2$ is the kinetic energy operator, $U(x)$ is the time independent potential energy at the position x and $\psi(x,t)$ is the wave function.

Here m is representing the mass of the particle and ∇^2 is the Laplace operator.

We can write equation (1) for the general quantum system as,

$$i\hbar\frac{\partial}{\partial t}\psi=\widehat{H\psi} \tag{2}$$

where, $\widehat{H}=-\frac{\hbar^2}{2m}\nabla^2+U(x)$ is the Hamiltonian operator for a single particle in a potential $u(x)$, $\hbar$ is the Planck's constant and $\widehat{H}$ is the Hamiltonian operator.

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2. OUTLINE OF THE GALERKIN FINITE ELEMENT METHOD

For a variational method of the SE,

$$(\widehat{H}-\lambda)\psi = 0 \tag{3}$$

By using this method we need two things. They are,

1. Choose a Basis or Shape function ϕ_i for the approximation of the solution,

$$U_h = \sum_{i=1}^{N} \xi_i \phi_i \tag{4}$$

where, ξ_i are the element parameters and ϕ_i are the shape functions.

2. To find the unknowns parameters ξ_i is a general matrix eigenvalue problem $(H_{ij} - \lambda^M S_{ij})\xi_j = 0$ has to be solved. Where,

$$H_{ij} = \int_\Omega \phi_i(\widehat{H}\phi_j)d\Omega \tag{5}$$

$$S_{ij} = \int_\Omega \phi_i\phi_j d\Omega \tag{6}$$

To apply the finite element method to the SE, the infinite solution domain $\tilde{\Omega}$ should be truncated to a finite volume Ω. Finite volume Ω is chosen to be sufficiently large. So, the solution in $\tilde{\Omega}\backslash\Omega$ can be assumed to be zero without affecting the eigen values.

3. NUMERICAL RESULTS

Let us consider the eigen value problem,

$$\begin{aligned} -\triangle u + cu &= \lambda u \quad \text{in} \quad \Omega \\ u &= 0 \quad \text{on} \quad \partial\Omega \end{aligned} \tag{7}$$

We seek the approximation $U_h(x,t)$ to the solution $u(x,t)$

Multiply equation (7) by a function of $w \in H_0^1(\Omega)$ are integrate over Ω. After integration by parts, we obtain the weak formulation of equation (7).

Find $u \in H_0^1(\Omega)$ and $\lambda \in \mathbb{R}$ such that,

$$\int_\Omega Du.Dwdx + \int_\Omega cuwdx = \int_\Omega \lambda uwdx \quad \text{for all,} \quad w \in H_0^1(\Omega) \tag{8}$$

Let $L = -\triangle + c$

L is representing the self-adjoint if c is positive and has an orthonormal basis of eigenfunctions $\{W_i\}_{i=1}^{\infty}$ and a corresponding sequence of eigenvalues $\{\lambda_i\}_{i=1}^{\infty}, 0 < \lambda_1 < \lambda_2 ...$

Now we need to define a mesh $\tau_h \subseteq \Omega$

Let, $W_h = \{w \in C(\Omega) : w/K_h \text{ linear}, w = 0 \text{ on } \partial\Omega\}$, k_h being trianlges in two dimensioanl and subintervals in one dimension. Ω is a convex polygon in two dimension and an interval in one dimension.

We choose a basis function in $W_h, \{\varphi_i\}_{i=1}^N$ so that, $W_h = \text{span } \{\varphi_i\}_{i=1}^N$

Further we let,

$$U_h = \sum_{i=1}^{N} \xi_i \varphi_i \tag{9}$$

Weak FEM formulation

Find $u_h \in W_h$ and λ_h such that,

$$\int_\Omega Du_h \cdot Dwdx + \int_\Omega cu_h wdx = \int_\Omega \lambda_h u_h wdx \qquad \text{for all } w \in W_h \tag{10}$$

If we insert equation (9) into equation (10) we get, with the choice $w = \varphi_j$, $j = 1, ..., N$;

$$\int_\Omega D\left(\sum_{i=1}^{N}\xi_i\varphi_i\right)\cdot D\varphi_j dx+\int_\Omega c\left(\sum_{i=1}^{N}\xi_i\varphi_i\right)\varphi_j dx=\int_\Omega \lambda_h\left(\sum_{i=1}^{N}\xi_i\varphi_i\right)\varphi_j dx \tag{11}$$

Interchanging sum and integration, we can write this as,

$$\sum\xi_i\int_\Omega\left[D\varphi_i\cdot D\varphi_j dx+\int_\Omega c\varphi_i\cdot\varphi_j dx\right]=\lambda_h\sum\xi_i\int_\Omega\varphi_i\varphi_j dx, \qquad j=1,...,N \tag{12}$$

with,

$$A_{ij}=\int_\Omega D\varphi_i\cdot D\varphi_j dx \tag{13}$$

$$Mc_{ij}=\int_\Omega c\varphi_i\varphi_j dx \tag{14}$$

$$M=\int_\Omega \varphi_i\varphi_j dx \tag{15}$$

$\xi=(\xi_1,...,\xi_N)$
After substituting these, we get equation (12) as,

$$[A+Mc]\xi=\lambda_h M\xi \tag{16}$$

and from equation (16),

$$M^{-1}[A+Mc]\xi=\lambda_h\xi \tag{17}$$

We can solve this matrix eigenvalue problem in Matlab as,

$$\lambda_h=eig(M^{-1}[A+Mc]) \tag{18}$$

where λ_h represent the eigenvalues.

4. ERROR ESTIMATES

The error estimates for the computed eigenvalues and eigenfunctions are,

$$0\leq\lambda_h-\lambda\leq c\parallel hD^2u\parallel^2_{L^2(\Omega)} \tag{19}$$

$$\parallel u-u_h\parallel_{L^2(\Omega)}\leq c\left(1+\frac{2\lambda}{d}\right)\parallel h^2D_h^2\parallel_{L^2(\Omega)} \tag{20}$$

where, d is the distance between λ which is the closest neighbour eigenvalues.

Let us start with Schrödinger equation for a particle with mass m in a potential $V=V(x)$.

$$i\hbar\frac{\partial\psi}{\partial t}=-\frac{\hbar^2}{2m}\triangle\psi+V\psi \tag{21}$$

By using a method of separation variable,

$$\psi(x,t)=u(x)v(t) \tag{22}$$

which leads to,

$$-\frac{\hbar^2}{2m}\triangle u\cdot v+Vuv=i\hbar\frac{\partial v}{\partial t}u \tag{23}$$

Dividing by uv in equation (23) we get,

$$-\frac{\hbar^2}{2mu}\triangle u\cdot + V = \frac{i\hbar}{v}\frac{\partial v}{\partial t}(t) = E \tag{24}$$

Finally we obtained the following two equations,

$$-\frac{\hbar^2}{2m}\triangle u\cdot + Vu = Eu \tag{25}$$

$$i\hbar\frac{\partial v}{\partial t}(t) = Ev \tag{26}$$

Equation (25) is the eigenvalue problem for the time independent Schrödinger equation, and it is of the same types as of equation (7). The quantity $H = -\frac{\hbar^2}{2mu}\triangle + V$ is called the Schrödinger Hamiltonian.

5. SOLUTIONS OF EIGEN VALUES

Consider the problem of finding the eigenvalues (λ) such that,

$$-u'' + x^2u = \lambda u \qquad [-8,8] \tag{27}$$
$$u(-8) = u(8) = 0$$

The exact solution of the above problem is,

$$\lambda_1 = 1$$

$$\lambda_2 = 3$$

$$\lambda_3 = 5$$

$$\lambda_4 = 7$$

To find the eigenvalues of equation (27), we apply a 1-dimensional FEM-program.

Simulations were performed with uniform meshes on [-8, 8] with the interval length $h = 0.1$, $h = 0.01$ and $h = 0.001$.

The following results were obtained finally as shown in table 1.

Table 1.Eigenvalues corresponding to the eigenmodes

h	λ_1	λ_2	λ_3	λ_4
0.1	1.00145	3.00401	5.00900	7.01642
0.01	1.0000	3.00000	5.00012	7.00021

For the two dimensional case, consider the eigenvalue problem in the plane

$$\begin{cases} -\triangle u = \lambda u & on \quad \Omega \\ u = 0 & on \quad \partial\Omega \end{cases} \tag{28}$$

where Ω is a unit circle entered at origin.

We calculated the first six eigen modes of vibration of a drum and by finite element method, obtained the following result as shown in table 2 given below.

Table 2.Eigenvalues corresponding to the eigenmodes

Eigen mode	1	2	3	4	5	6
Eigen value	5.80144	14.78833	14.79295	26.73301	26.73892	30.93363

It is to be noted that the first eigenvalue in the above table is simple but the second and the third are doubled.

The eigen values obtained with the potential were in close agreement with the eigen values obtained without potential.

It is concluded that the accurate scaling of the quantum oscillator have to select the large potential, in comparison with the Laplace term.

Example

Quantum harmonic oscillator in two dimensional case

$$\begin{cases} -\triangle u + (y_1^2 + y_2^2)u = \lambda u & on \quad \Omega \\ u = 0 & on \quad \partial\Omega \end{cases}$$

The following numerical results are obtained as shown in table 3.
Result = 1.0e+02*

Table 3.Eigenvalues corresponding to the eigenmodes

Eigenmode	1	2	3	4	5	6
Eigenvalue	0.64333	1.29575	1.29812	1.95701	1.95912	1.97274

Consider the eigen value problem for very large potentials,

$$-\frac{\hbar^2}{2m}\triangle u + (y_1^2 + y_2^2)u = \lambda u$$

$$i. -\triangle u + 10^3(y_1^2 + y_2^2)u = \lambda u$$

$$ii. -\triangle u + 10^6(y_1^2 + y_2^2)u = \lambda u$$

$$iii. -\triangle u + 10^9(y_1^2 + y_2^2)u = \lambda u$$

After applying the FEM we obtained the following results,

i.Result = 1.0e+02*

Eigenmode	1	2	3	4	5	6
Eigenvalue	0.64333	1.29574	1.29812	1.95701	1.95912	1.97273

ii.Result = 1.0e+4*

Eigenmode	1	2	3	4	5	6
Eigenvalue	0.38521	0.87422	0.99804	1.32221	1.37222	1.83674

REFERENCES

[1] R.Shankar, Principles of Quantum Mechanics, Springer Science & Business Media, Germany, 2012, pp. 1-696.

[2] Mehar Chand, Sequence of Functions involving the Product of S-Functions, DJ Journal of Engineering and Applied Mathematics, Vol. 2, No. 2, 2016, pp. 15-23, http://dx.doi.org/10.18831/djmaths.org/2016021003.

[3] D.R.Bes, A brief History of Quantum Mechanics. Quantum Mechanics: A Modern and Concise Introductory Course, Springer, Germany, 2007, pp. 201-214.

[4] Archit Yajnik and Rustam Ali, Numerical Solution of Integral Equations by using Discrete GHM Multi-Wavelet, DJ Journal of Engineering and Applied Mathematics, Vol. 1, No. 1, 2015, pp. 17-22, http://dx.doi.org/10.18831/djmaths.org/2015011003.

[5] Nitin Ramchandra Gadre, Mathematical Model I. Electron and Quantum Mechanics, AIP Advances, Vol.1, No. 1, 2011, http://dx.doi.org/10.1063/1.3559460.

[6] Azhar Iqbal, Some Aspects on the Schrödinger Equation, Master's Thesis, Chalmers University of Technology and University of Gothenburg, Sweden Gothenburg, 2012.

[7] F.A.Berezin and M.Shubin, The Schrödinger Equation, Springer Science & Business Media, Germany, 2012.

[8] J.Ackermann and R.Roitzsch, A Two Dimensional Multilevel Adaptive Finite Element Method for the Time Independent Schrödinger Equation, Chemical Physics Letters, Vol. 214, No. 1, 1993, pp. 109-117, https://doi.org/10.1016/0009-2614(93)85463-X.

[9] S.Y.Cheng and P.Li, Heat Kernel Estimates and Lower Bound of Eigenvalues, Commentarii Mathematici Helvetici, Vol. 56, No. 1, 1981, pp. 327-338.