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On the Numerical Solution Of Schrodinger Equation

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Abstract

In the beginning, we start with reviewing basic concepts such as inner product and Hilbert spaces; then we introduce Schrodinger Equation(SE)focusing on the solution of time–dependent and time–independent SE with a stress on the harmonic oscillator (HO) problem which will be the ingredient for our subject ; namely, the numerical solution of SE.
The numerical solution of SE is then tackled using the so–called potential morphing method(PMM). Calculations were carried out for the ground state of the HO which represents the frame of reference to work with. The obtained results were compared with similar ones and found to be in very good agreement. Finally, a brief discussion related to possible future work is given; moreover recent works on the subject are exposed to .

Keywords:

Numerical , Solution , Schrodinger Equation , Potential Morphing Method .

1. Introduction

As we know getting exact solutions, or solutions in closed forms , of Schrodinger equation for some important problems in physics, is possible .However ,there is no general method to obtain these solutions and the reader should always be acquainted with the methods of solving partial differential equations. We should add that many problems cannot be solved analytically, hence numerical solutions for SE are needed . Accordingly, this paper came into light.
In the next section, we give basic concepts related to inner product and Hilbert spaces, then in section 3,we introduce SE focusing on the mathematical solution of the HO problem [1].
In section 4, we introduce the numerical solution of SE for a particle under a general potential discussing the use of different techniques [2][3].In the same section, we introduce the PMM and its application to the simple harmonic oscillator(SHO) problem[3]. In section 5, we give the results of our calculations [2]; and in the last section, we conclude with brief remarks about possible future work and recent results on the subject [4], [5], [6].

2. Basic concepts

Definition 1

Given the two vectors $\vec{u} = (x_1, x_2, \dots, x_n)$ and $\vec{v} = (y_1, y_2, \dots, y_n)$ in the space $\mathbb{R}^n$ then the inner product of the two vectors $\vec{u}$and $\vec{v}$is

$$\vec{u} \cdot \vec{v} = \sum_{i=1}^{n} x_i y_i \tag{1}$$

The inner product defined by Equation(1) has the following properties [7]

$(i)\vec{u}.\vec{v} \geq 0$
$(ii)\vec{u} = 0 \Leftrightarrow \vec{u}.\vec{u} = 0$
$(iii)\vec{u}.0 = 0$
$(iv)\vec{u}.\vec{v} = \vec{v}.\vec{u}$
$(v)\vec{u}.(\vec{v} + \vec{\omega}) = \vec{u}.\vec{v} + \vec{u}.\vec{\omega}$
$(vi)(\vec{u} + \vec{v}).\vec{\omega} = \vec{u}.\vec{\omega} + \vec{v}.\vec{\omega}$
$(vii)(\alpha\,\vec{u}).\vec{v} = \alpha(\vec{u}.\vec{v})$
$(viii)\vec{u}.(\alpha\vec{v}) = \alpha(\vec{u}.\vec{v})$
) (where$\vec{u}, \vec{v}, \vec{\omega} \in \mathbb{R}^nand\alpha \in \mathbb{R}$

Definition 2

Given the two vectors $\vec{u}$and $\vec{v} \in \mathbb{R}^n$ the norm of $\vec{u}$is defined as

$$\|\vec{u}\| = \sqrt{\vec{u}.\vec{u}} = \sqrt{x_1^2 + x_2^2 + \cdots, +x_n^2} \tag{2}$$

Moreover ,the distance between the two vectors $\vec{u}$and $\vec{v}$ is given by

$$d(\vec{u}, \vec{v}) = \|\vec{u} - \vec{v}\| = \sqrt{(x_1 - y_1)^2 + (x_2 - y_2)^2 + \cdots + (x_n - y_n)^2} \tag{3}$$

One can also get the unit vector for any non-zero vector $\vec{u}$ as

$$\hat{u} = \frac{\vec{u}}{\|\vec{u}\|} \tag{4}$$

Definition 3

The vector space V is a function the inner product on
$V \to \mathbb{R} : \langle -, - \rangle$for every ordered pair $\vec{u}, \vec{v} \in V$ such that $\langle \vec{u}, \vec{v} \rangle$ is a real number
and satisfies the following conditions:

(i)$\langle \vec{u}, \vec{v} \rangle \geq 0$ and $\vec{u} = 0 \Leftrightarrow \langle \vec{u}, \vec{u} \rangle = 0$.
(ii)$\langle \vec{u}, \vec{v} \rangle = \langle \vec{v}, \vec{u} \rangle \; \forall \, \vec{u}, \vec{v} \in V$.
(iii)$\langle \vec{u}, \vec{v} + \vec{\omega} \rangle = \langle \vec{u}, \vec{v} \rangle + \langle \vec{u}, \vec{\omega} \rangle$
(iv) $\alpha\langle \vec{u}, \vec{v} \rangle = \langle \alpha\vec{u}, \vec{v} \rangle \; \forall$ scalars α .

V with the inner product operation is called an inner-product space .

Definition 4

A space is complete if every Cauchy sequence in that space is convergent to an element in the space ,and any infinite – dimensional complete space is called a Hilbert space [8].

Note that if f, g, h , ... belonging to a Hilbert space H ,then H satisfies the following conditions :

(i) H is a Euidean space .

(ii) H is complete with the distance defined as

$$d(f, g) = \|f - g\| \tag{5}$$

(iii) the dimension of H is infinite.
(iv) H is seperable .
(Note that the eigenfunctions obtained by solving SE form a Hilbert space)

3. Schrodinger Equation

The time-dependent Schrodinger equation is written as

$$i\hbar \frac{\partial \psi}{\partial t} = \left[-\frac{\hbar^2}{2m}\nabla^2 i + V(r)\right]\psi \tag{6}$$

or as

$$i\hbar \frac{\partial \psi}{\partial t} = \widetilde{H}\psi \tag{7}$$

where ψ is the wave function and H is the Hamiltonian given by
$\widetilde{H} = -\frac{\hbar^2}{2m}\nabla^2 + V$;this equation is solved using separation of variables. Note that $i\hbar \frac{\partial}{\partial t}$ is the energy operator[9]; and that the solution is obtained in a closed formwhen the potential is a simple one. However ,to get the solution, in general ,is a difficult job .Hence, one refers to numerical methods .
To add, the time–independent Schrodinger equation is given by

$$-\frac{\hbar^2}{2m}\nabla^2\psi(r) + V(r)\psi(r) = E\,\psi(r) \tag{8}$$

where E is the energy eigenvalue .

3.1 Schrodinger Equation for the Simple Harmonic Oscillator

The SE for the simple harmonic Oscillator (SHO) in one dimension can be written as

$$\frac{d^2\psi}{d\zeta^2} + (\varepsilon - \zeta^2)\psi = 0 \tag{9}$$

where $\zeta = \sqrt{\frac{1}{2}\,k\,x^2}$ and ε is the energy eigenvalue .The last equation was written in a simple form through a sequence of substitutions [10].
Now, using finite difference method one obtains the difference equation

$$\psi_{j+1} = [2 - (h)^2(\varepsilon - (jh)^2)]\psi_j + \psi_{j-1} = 0 \tag{10}$$

where h is the step length .Taking $\psi_1 = \psi_2 = 1$, $h = 0.01$ and $\varepsilon = 5.01404$, one gets the wave function and the probability density for the HO as is shown in Figure 1

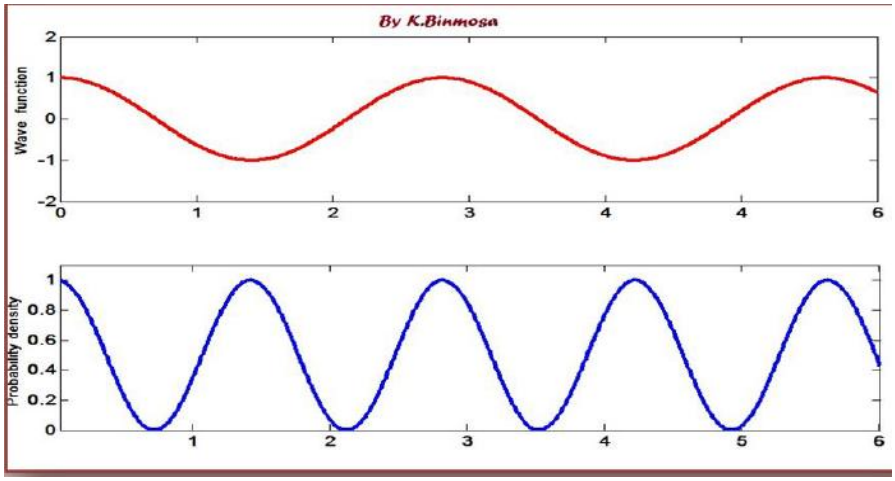

Figure 1 . The wave function and probability density for the HO ($h = 0.01$, $\varepsilon = 5.01404$)

Example 1

To solve the equation $-u'' + x^2 u = \lambda u$ (λ is the eigenvalue), we put $u = e^{-x^2/2} y$ to get $y'' - 2xy' + 2ny = 0$, with $\lambda = 2n + 1$ and y is then given by $y = H_n(x)$ where $H_n(x)$ are Hermite polynomials. Table 1 shows the eigenvalues(energies) for the HO.

$\left[\text{Note that } \eta = \hbar , x = \sqrt{\frac{\hbar}{m\omega}}\ \zeta \text{ am } E = (E_n) = \frac{1}{2}\hbar\omega_0\varepsilon \right]$.

Table 1 . The energy eigenvalue for the HO .

N	Exact Value	En	$H_n(x)$
0	1	$\frac{1}{2}\hbar\omega$	1
1	3	$\frac{3}{2}\hbar\omega$	2y
2	5	$\frac{5}{2}\hbar\omega$	$4y^2+2$
3	7	$\frac{7}{2}\hbar\omega$	$8y^3-12y$
4	9	$\frac{9}{2}\hbar\omega$	$16y^4-48y^2$
5	11	$\frac{11}{2}\hbar\omega$	$32y^5-160y^3+120y$

Moreover, we present the HO potential and wave functions in Figure 2 [10].

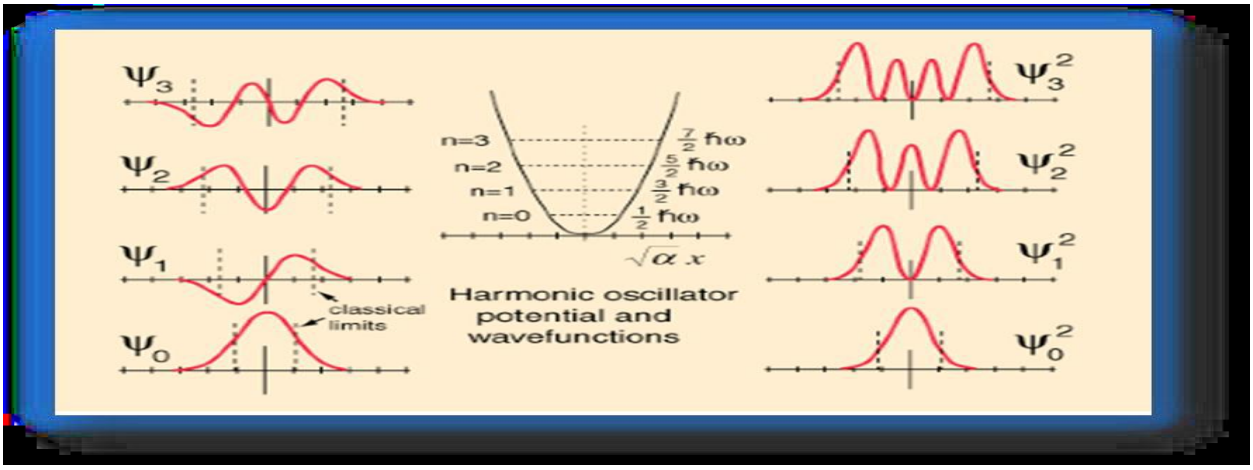

Figure 2.Potential and wave functions for the HO [10].

4. Numerical Solution of Schrodinger Equation for a particle under a General Potential

In this section, we repeat numerical calculations obtained through the use of a novel method from which the eigenvalues and eigenfunctions were calculated for a particle (an electron say) under a general–shape potential [3].

To begin with ,we should note that the numerical solutions in solving Schrodinger equation are necessary only when the solutions are not possible analytically. One can use perturbation techniques, variational methods, or other methods which depend on diagolaniztion and finite–element methods [2].However we shall deal here with a novel method which uses a so–called morphing potential [3]; writing Schrodinger equation as

$$\left(\frac{-\hbar^2}{2m}\nabla^2 + v_s(r)\right)\psi_s(r) = E_s\psi_s(r) \tag{11}$$

whereE_s is the eigenvalue corresponding to the eigenfunctionψ_s ; s represents the reference system under study and$v_s(r)$is the potential.

If we assume, now, that we have another reference system R, in which the different quantities are known , then

$$\left(\frac{-\hbar^2}{2m}\nabla^2 + v_R(r)\right)\psi_R(r) = E_R\psi_R(r) \tag{12}$$

and transferring from the system R to that of S, one refers to the time – dependent Schrodinger equation as

$$\hbar\,\frac{\partial\psi(r,t)}{\partial t} = \left(\frac{-\hbar^2}{2m}\nabla^2 + v_t(r)\right)\psi(r,t) \tag{13}$$

with the potential $v_t(r)$ given by

$$v_t(r) = \sigma(t)v_s(r) + [1 - \sigma(t)]v_R(r) \tag{14}$$

and

$$\sigma(t) = \begin{cases} 0 & t \leq t_a \\ 1 & t \geq t_b \end{cases} \tag{16}$$

Using Equation (13) along with the next two equations, we get [3]

For

$$t \leq t_a \quad : \quad \psi(r,t) = \psi_R(r,t) = C_R \exp\left(\frac{-i}{\hbar} E_R\, t\right) \psi_R(r) \tag{17}$$

and

For

$$t \geq t_b \quad : \quad \psi(r,t) = \psi_s(r,t) = C_s \exp\left(\frac{-i}{\hbar} E_s\, t\right) \psi_s(r) \tag{18}$$

To integrate Equation (13) , we need to divide the time interval $t_b - t_a$ to N subintervals, i.e. , $\Delta t = \frac{t_b - t_a}{N}$; then we get

$$\psi(r,t_1) - \psi(r,t_a) = \frac{1}{i\hbar}\int_{t_a}^{t_1}\left(\frac{-\hbar^2}{2m}\nabla^2 + v_t(r)\right)\psi(r,t)\,dt \tag{19}$$

where $t_1 = t_a + \Delta t$ and $\psi(r,t_a)$ refers to the wave function in system R , i.e.

$$\psi(r,t_a) = \psi_R(r,t) \tag{20}$$

Note that the perturbation in $\psi(r\,,t)$ is given by

$$\delta\psi(r,t) = \frac{1}{i\hbar}\int_{t_a}^{t_1}\left(\frac{-\hbar^2}{2m}\nabla^2 + v_t(r)\right)\psi(r,t)\,dt \tag{21}$$

Assuming that we can make $\delta\psi(r,t) \to 0$, then we can put $\psi(r,t) \approx \psi(r,t_a)$ in the calculation ; moreover , even though $v_S(r)$ is very much different from $v_R(r)$, for large N one can make $v_t(r) \approx v_R(r)$, e.g .if $N = 10^3$,we get [3]

$$v_t(r) = 10^{-3}\, v_s(r) + 0.999\, v_R(r) \tag{22}$$

The second step in the recursive operation is

$$\psi(r,t_2) = \psi_R(r,t_a) + \delta\psi(r,t_1) + \frac{1}{i\hbar}\int_{t_1}^{t_2}\left(\frac{-\hbar^2}{2m}\nabla^2 + v_t(r)\right)\psi(r,t)\,dt \tag{23}$$

where $t_2 - t_a = 2\Delta t$.

To compute the integral in the last equation , we have to use Equation (19) for $\psi(r, t_1)$ and for N recursive steps ,we get [3]

$$\psi(r, t_N) = \psi_R(r, t_a) + \sum_{k=1}^{N} \delta\psi(r, t_k) = \psi(r, t_b) \quad (24)$$

When $t \geq t_b$

$$\psi_s(r) = \psi_s(r, t_b) \quad (25)$$

$\psi_s(r)$ satisfies Equation (11) as pointed out before. Moreover E_s is obtained as [3]

$$E_s = \int_{-\infty}^{\infty} \psi_s^*(r) \left(\frac{-\hbar^2}{2m} \nabla^2 + v_s(r) \right) \psi_s(r)\, dr \quad (26)$$

Note that every wave function obtained in the recursive process satisfies Schrodinger equation; for instance after ten steps of recursion we have [2][3]

$$\left(\frac{-\hbar^2}{2m} \nabla^2 + \frac{10}{N} v_S(r) + \left(1 - \frac{10}{N}\right) v_R(r) \right) \psi(r, t_{10}) = E_{10}\, \psi(r, t_{10}) \quad (27)$$

Using this method, the reference system R with potential $v_R(r)$ will escalate, with time, to the system S with potential $v_S(r)$; for this reason this method was called the potential morphing method [3].

To clarify the ideas presented so far, we give for simplicity the calculation for the harmonic oscillator in one dimension. In this case we choose

$$v_R(x) = \frac{1}{2} m \omega_0^2 x^2 \quad (28)$$

and

$$v_S(x) = \frac{1}{2} m(\omega_0^2 + \omega_p^2) x^2 \quad (29)$$

The term containing ω_p^2 can be considered as a perturbation [11]; and transferring from $R\ with\ v_R(r) to\ S\ with\ v_S(r)$ is accomplished by using the potential morphing method [3] .

Using Equation (28) and writing the Hamiltonian as

$$H \equiv \frac{-\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{1}{2} m \omega_0^2 x^2 \quad (30)$$

with a simple transformation of coordinates ,$x = a\, y$, and putting $\frac{m_0^2 \omega_0^2 a^4}{\hbar^2} = 1$, we get the equation [3]

$$\left(-\frac{d^2}{dy^2} + y^2 \right) \psi = 2\psi \quad (31)$$

Hence $H_R = -\frac{d^2}{dy^2} + \frac{1}{2}y^2$ and $v_R = \frac{1}{2}y^2$.

Moreover , we get $H_S = -\frac{1}{2}\frac{d^2}{dy^2} + y^2$, $V_S = y^2$;and where we put $\omega_0^2 = \omega_p^2$.

Equation (14) takes, then, the form

$$v_t(y) = \frac{\delta}{\delta_b}y^2 + \left(1 - \frac{\delta}{\delta_b}\right)\frac{1}{2}y^2 \tag{32}$$

Also, we have

$$i\frac{\partial\psi}{\partial t} = \{ -\frac{d^2}{2\,dy^2} + \left[\frac{\delta}{\delta_b}y^2 + \left(1 - \frac{\delta}{\delta_b}\right)\frac{1}{2}y^2\right] \}\,\psi \tag{33}$$

Now, for the simple harmonic oscillator

$$\psi(y) = e^{-y^2/2} \tag{34}$$

and if we use Runge–Kutta method of the fourth order [2] [3] , to solve the equation

$$\frac{\partial\psi}{\partial t} = f(y,\tau) \tag{35}$$

we get

$$i\left(\frac{\psi(x+\Delta x,t)+\psi(x-\Delta x,t)-2\psi(x,t)}{2(\Delta x)^2} - v(x)\,\psi(x,t)\right) = f(x,\psi) \tag{36}$$

5 . Results

To perform the calculations, the following quantities need to be calculated , i.e.

$$k_1 = f(\psi_n)\,,\quad k_2 = f\left(\psi_n + \frac{1}{2}\Delta\tau\,, k_1\right)\,, k_3 = f\left(\psi_n + \frac{1}{2}\Delta\tau\,, k_2\right),$$

$$k_4 = f(\psi_n + \Delta\tau\,, k_3)$$

To get the recurrence relation

$$\psi_{n+1} = \psi_n + \frac{1}{6}\Delta\tau\,(k_1 + 2k_2 + 2k_3 + k_4) \tag{37}$$

Figure 3 shows our results for the case of $\omega_p^2 = \omega_0^2$ [2] .

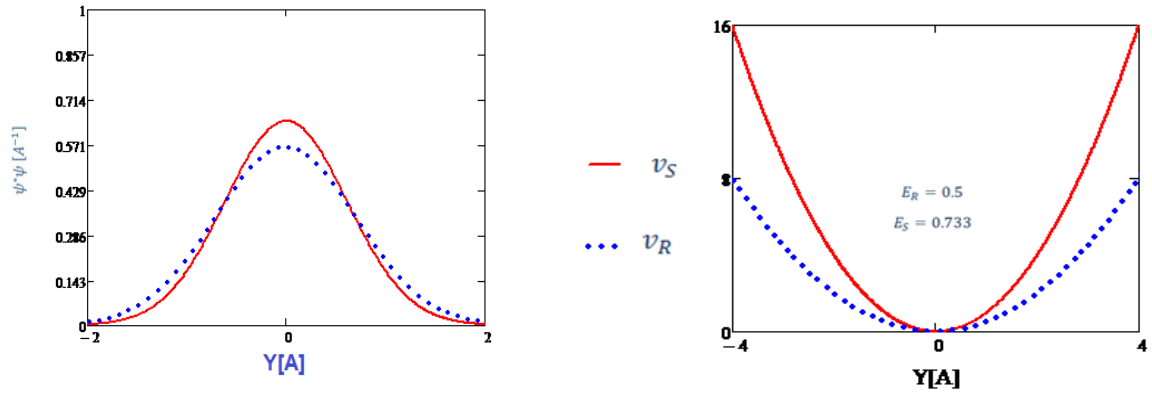

Figure 3 . The probability density $\Psi^*\Psi$ versus y for $\omega_p^2 = \omega_0^2$ when $E_R = 0.5$ and $E_S = 0.733$.

Figure 4 , Figure 5 and Figure 6 give similar results as in Figure 3 for$\omega_p^2 = 0.1\omega_0^2$, $\omega_p^2 = 0.5\ \omega_0^2$and $\omega_p^2 = 0.75\ \omega_0^2$ respectively .

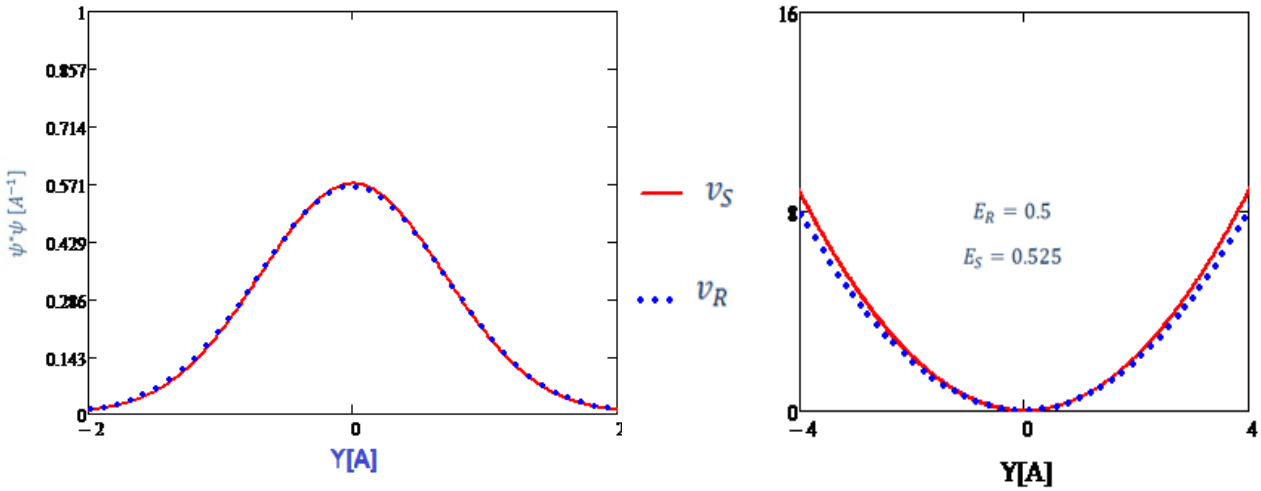

Figure 4 . The probability density $\Psi^*\Psi$ versus y for $\omega_p^2 = 0.1\ \omega_0^2$($E_R = 0.5$, $E_S = 0.525$)

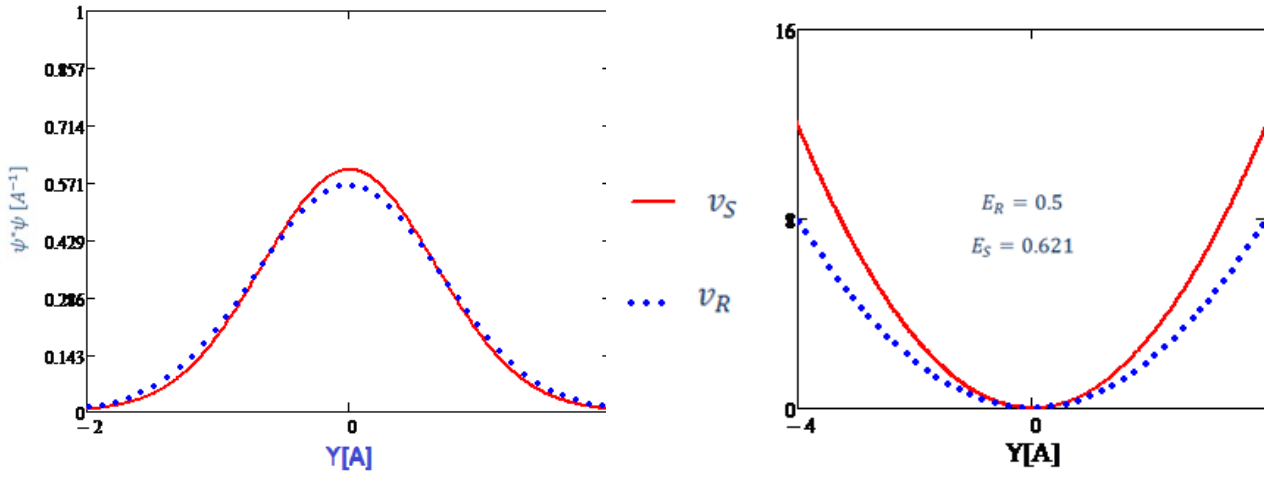

Figure 5 . The probability density $\Psi^*\Psi$ versus y for $\omega_p^2 = 0.5\ \omega_0^2$($E_R = 0.5$, $E_S = 0.621$)

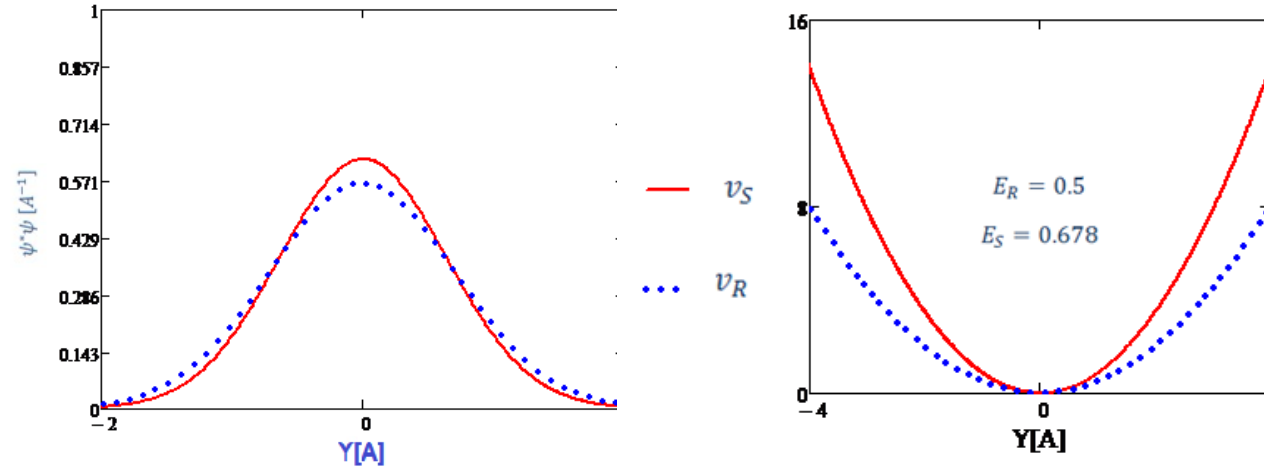

Figure 6 . The probability density $\Psi^*\Psi$ Versus for $\omega_p^2 = 0.75\ \omega_0^2$($E_R = 0.5$, $E_S = 0.678$)

Note that the calculations were carried out using the potential morphing method for the ground state of the simple harmonic oscillator and our calculations agreed very well with the previous work on the subject [2] [3].

6. Concluding Remarks

The potential morphing method proved to be a very good method in solving Schrodinger equation numerically [2] [3]. In the present work our result were given for the ground state of the simple harmonic oscillator just for simplicity , but the method can be extended to include calculations for higher excited states for the simple harmonic oscillator ,as was shown earlier [3] ,and to include other examples .Moreover ,one can use perturbation theory to perform calculations on the same line [11] .

Recently, quite a good number of research articles were published on the numerical solution of Schrodinger equation. To mention a few, an article was written on the analytical and numerical solutions of the one–dimensional nonlinear Schrodinger equation where four numerical approaches ; the split–step Fourier transform ,Fourier pseudo spectral method, Crank – Nicolson ,and Hopscotch method , were presented in details for solving nonlinear Schrodinger equation in one dimension [4] .

The behavior of numerical solutions for a nonlinear eigenvalue problem on $\mathbb{R}^n$ in conjunction with dispersion managed solutions where a finite difference scheme is implemented [5].

A family of numerical methods were constructed for the Pauli equation of charged particles in a time–dependent, homogeneous magnetic field ;the methods were described in a general setting [6].

Another somewhat recent paper was written on numerical long–time energy conservation for the nonlinear Schrodinger equation; the paper investigated the long–time near–conservation of energy via the spit–step Fourier method applied to the cubic nonlinear SE on a torus [12].

From the fore–mentioned papers, we conclude that there is always a need for numerical schemes to get the solutions of SE once the analytic solutions are not attainable.

References

[1] Mathews, P.(1968) Introduction to Quantum Mechanics, 2nd Edition, McGraw Hill , London .

[2] Ben Mussa,K.A.(2014) The Numerical Solution of Schrodinger Equation, MSc . Thesis, University of Tripoli, Tripoli.

[3] Rieth,M., Schommers, W.(2002) Novel Numerical Method for the Solution of Schrodinger Equation: A Particle in an Interaction Potential of General Shape, International Journal of Modern Physics,B16,4081-4092 .

[4] Faraj, N .G.A., Eltanboly, A.H.,El-Azab, M.S.,Obayya,S.S.A.(2021) On the Analytical and Numerical Solutions of the One –Dimensional Nonlinear Schrodinger Equation, Mathematical Problems in Engineering, Article I D 3094011.

https: //doi.org /10.1155/2021/3094011

[5] Kang,Y.,Lee,E.,Lee,Y–R.(2021) Numerical Solutions for one and Two Dimensional Nonlinear Problems Related to Dispersion Managed Solitons, Journal of the Korean Mathematical Society,58,4,835-847 .

https://doi.org/10. 4134 /JKMS.j 200257

[6] Gradinaru,V.,Rietmann,O.(2020) A High–Order Integrator for the Schrodinger Equation with Time–Dependent Homogeneous Magnetic Field, SMAI Journal of Computational Mathematics,6,253 -271.

[7] Barnett,R.,Ziegler,M.R.(2010) Linear Algebra,9th Edition, Ellen Publishing company, New York .

[8] Debnath,L., Mikusinski,P.(2005) Introduction to Hilbert Spaces,1st Edition , Elsevier–Academic Press, New York .

[9] Le Veque,R.(2007) Methods for Ordinary and Partial Differential Equations : Steady–State and Time–Dependent Problems, Society for Industrial and Applied Mathematics (SIAM), Philadelphia .

[10] Al-Rabadi,A.(2009)Closed-System Quantum Logic Network Implementation of the Viterbi Algorithm,FACTA UNIVERSITATIS Series Electronics and Energetics, DOI:10.2298/FUEE0901001A.

https://www.researchgate.net/publication/228529042

[11] Awin,A.A.,Sharif,B.W.,Awin,A.M.(2021) On the Use of Perturbation Theory in Eigenvalue Problems,Journal of Applied Mathematics and Physics,9, 2224-2243 .

https://doi.org/10.4236/jamp.2021.99142

[12] Gauckler,L.(2017) Numerical Long-Time Energy Conservation for the Nonlinear Schrodinger Equation, IMA Journal of Numerical Analysis,37,2067 -2090.