SOLVING THE HARMONIC AND ANHARMONIC OSCILLATORS WITH MATRIX METHOD

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Abstract

Attempts have been made to investigate a simple technique for solving the Schrödinger equation. This involved Matrix formulation of time independent Schrödinger equation, matrix representation of position and momentum operators, harmonic oscillators and anharmonic oscillators. Then, the numerically exact Eigen values (i.e. the possible results of a measurement of energy) and Eigen vectors for models have been investigated through matrix method and relevant numerical simulations have been implemented using Mathematica coding.

Keywords: Matrix method, Schrödinger equation, Mathematica coding

Introduction

One of the most fundamental theories of physics is quantum mechanics. The behavior of matter and energy on the scale of atomic and subatomic particles or wave can be explained by quantum mechanics. In quantum mechanics the wave function, also talk about the state function, is taken to be the most complete description that can be assigned to a physical system (Sakurai, J.J., 1994). The Schrödinger equations solutions are very useful to describe the behavior of microscopic system, macroscopic system and in all probability the entire universe. The Eigen functions are carefully chosen from a special class of functions. So, the general solutions of harmonic and shift harmonic oscillator have a very interesting property that each Eigen function is linked with a particular Eigen energy value of each potential (Kahn, K., 2008).

This research attention on the extension of the matrix mechanics but instead of just deriving a matrix method that can be used to solve an-harmonic oscillator with a general matrix expression. So, the Schrödinger equation is applied and the wavefunction is written in terms of another set of orthonormal basis wave functions. Then, the eigenvalue equation is derived. From here the matrix equation is found for the Hamiltonian operator. The target of this research now becomes to solve for this matrix equation, so as to get energy (eigenstates) and Eigen functions. So, the Hamiltonian is modified in the form of ladder operators and answered for the matrix elements for manufacture the whole process easy. The Hamiltonian matrix elements are solved with the help of Mathematica and Eigen function regardless of whether the matrix is diagonal or not.

Matrix formulation of time independent Schrödinger equation

Schrödinger equation is very useful equation in quantum mechanics that can solve the most fundamental problems. The time independent Schrödinger equation is

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+V(x)\right)\phi_n(x)=E\phi_n(x) \tag{1}$$

If the Hamiltonian is

$$H\phi_n(x)=E\phi_n(x) \tag{2}$$

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In the above condition, H , $\phi_n(x)$ indicated the Hamiltonian operator and the wave functions representing the state. Besides, the mass and the position are signified by *m* and *x* and the Eigen values or energy for the Hermitian operator is denoted by E_n (Franzke, M.C, et al, 2021). Then, the wavefunction $\phi_n(x)$ are rewritten by

$$\phi_n(x) = \sum_{i=0}^{\infty} c_i^{(n)} \psi_i(x) \tag{3}$$

Substituting in Equation (2) $\sum_{i=0}^{\infty} c_i^{(n)} H\psi_i(x) = E_n \phi_n(x)$

Multiplying both sides by $\psi_j^*(x)$ we have $\sum_{i=0}^{\infty} c_i^{(n)} \psi_j^*(x) H\psi_i(x) = E_n \psi_j^*(x) \phi_n(x)$. If $\int_R \psi_j^*(x) \phi_n(x)\, dx = c_j^{(n)}$, integrating above equation with respect to x over the R line

$$\sum_{i=0}^{\infty} c_i^{(n)} \int_R \psi_j^*(x) H\psi_i(x) dx = \int_R E_n \psi_j^*(x) \phi_n(x)\, dx = E_n \int_R \psi_j^*(x) \phi_n(x)\, dx$$

$$\sum_{i=0}^{\infty} c_i^{(n)} \int_R \psi_j^*(x) H\psi_i(x) dx = E_n c_j^{(n)} \tag{4}$$

Then H_{ji} is defined as $H_{ji} = \int_R \psi_j^*(x) H\psi_i(x)\, dx$

So, Equation (4) becomes, $\sum_{i=0}^{(n)} c_i^{(n)} H_{ji} = E_n c_j^{(n)}$ (5)

If *H* is chosen to be an $N \times N$ matrix, then *N* Eigenvalues and Eigen vectors will have. Specifically, *n* will go from 1 to *N* (Gupta, R., 2019,Okock, P. and Burns, T., 2015).

Ladder operators or creation and annihilation operators

To simplify the eigenvalue equation for time-independent Schrödinger equation, the two operators are introduced by

$$a_+ = \frac{1}{\sqrt{2}}(x - ip), \qquad a_- = \frac{1}{\sqrt{2}}(x + ip) \tag{6}$$

This pair are well known ladder operators with a_+ defined as the creation operator and a_- defined as the annihilation operator (Sakurai, J.J., 1994). Then, the number operator is defined as $N = a_+ a_-$, with eigenvalues *n* and Eigen functions $|n\rangle$. By the time ladder operators are rewritten in the form of position and momentum operator,

$$x = \frac{1}{\sqrt{2}}(a_+ + a_-) \qquad p = \frac{i}{\sqrt{2}}(a_+ - a_-) \tag{7}$$

So, the commutation relationships of raising and lowering operators developed

$$[a_-, a_+] = \frac{1}{2}[x+ip, x-ip] = \frac{1}{2}([x,-ip]+[ip,x]) = -i[x,p] = 1 \tag{8}$$

$$[N, a_-] = [a_+a_-, a_-] = [a_+, a_-]a_- = -a_- \tag{9}$$

$$[N, a_+] = [a_+a_-, a_+] = a_+[a_-, a_+] = a_+ \tag{10}$$

From the commutation relationships, $a_-|n\rangle = [a_-, N]|n\rangle = a_-n|n\rangle - Na_-|n\rangle$

$$Na_-|n\rangle = (n-1)(a_-|n\rangle) \tag{11}$$

where, N, $a_-|n\rangle$ and $(n-1)$ are operator, eigenvector (eigenstate) and eigenvalue. The annihilation operator $a_-|n\rangle$ is recognized by $a_-|n\rangle = c_n|n-1\rangle$. In the same way, $a_+|n\rangle$ is an eigenvector of N operator by Eigen value $(n+1)$: $a_+|n\rangle = [a_+, N]|n\rangle = a_+n|n\rangle - Na_+|n\rangle$

$$Na_+|n\rangle = (n+1)(a_+|n\rangle) \tag{12}$$

Therefore, the creation operator is recognized by $a_+|n\rangle = d_n|n+1\rangle$. Since $\langle n|N|n\rangle = \langle n|a_+a_-|n\rangle = n$ and $\langle n|a_+a_-|n\rangle = (\langle a_-n|)(a_-|n\rangle) = \langle n-1|n-1\rangle c_n^2$, $c_n = \sqrt{n}$.

Since $a_-a_+ = N+1$, from the commutation relationship:

$$d_n^2\langle n+1|n+1\rangle = \langle a_+n|a_+n\rangle = \langle n|a_-a_+|n\rangle\langle n|(N+1)|n\rangle = n+1 \tag{13}$$

So, $a_-|n\rangle = \sqrt{n}|n-1\rangle$, $a_+|n\rangle = \sqrt{n+1}|n+1\rangle$ and $N|n\rangle = n|n\rangle$. This three properties confirm with creation operator a_+, annihilation operator a_- and the number operator N yielded the quantum number n, for particles of the corresponding energy level (Sakurai, J.J., 1994).

Matrix representation of position and momentum operator

By applying the bra-ket notation, the position and momentum operator can be described

$$\hat{x}_{nm} = \langle n|x|m\rangle, \qquad \hat{p}_{nm} = \langle n|p|m\rangle \ . \tag{14}$$

Here the raising operator a_+ and lowering operator a_- will be useful. From Equation (7)

$$x = \frac{1}{\sqrt{2}}(a_+ + a_-) \ , \qquad \hat{x}_{nm} = \frac{1}{\sqrt{2}}(\langle n|a_-|m\rangle + \langle n|a_+|m\rangle) = \frac{1}{\sqrt{2}}(\langle a_+n|m\rangle + \langle n|a_+m\rangle)$$

$$\hat{x}_{nm} = \frac{1}{\sqrt{2}}\left(\langle\sqrt{n+1}\ n+1|m\rangle + \langle n|\sqrt{m+1}\ m+1\rangle\right)$$

$$\hat{x}_{nm} = \frac{1}{\sqrt{2}}\left(\sqrt{n+1}\delta_{n+1,m} + \sqrt{m+1}\delta_{n,m+1}\right) \tag{15}$$

By matrix representation, the position operator becomes

$$\hat{x} = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & \sqrt{1} & 0 & \cdots \\ \sqrt{1} & 0 & \sqrt{2} & \cdots \\ 0 & \sqrt{2} & 0 & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix} \tag{16}$$

Similarly $p = \frac{i}{\sqrt{2}}\left(a_+ - a_-\right)$, $\hat{p}_{nm} = \frac{i}{\sqrt{2}}\left(\langle n|a_+|m\rangle - \langle n|a_-|m\rangle\right) = \frac{i}{\sqrt{2}}\left(\langle n|a_+ m\rangle - \langle a_+ n|m\rangle\right)$

$$\hat{p}_{nm} = \frac{i}{\sqrt{2}}\left(\left\langle n\middle|\sqrt{m+1}\ m+1\right\rangle - \left\langle\sqrt{n+1}\ n+1\middle|m\right\rangle\right)$$

$$\hat{p}_{nm} = \frac{i}{\sqrt{2}}\left(\sqrt{m+1}\delta_{n,m+1} - \sqrt{n+1}\delta_{n+1,m}\right) \tag{17}$$

By matrix representation, the momentum operator become

$$\hat{p} = \frac{i}{\sqrt{2}} \begin{pmatrix} 0 & -\sqrt{1} & 0 & \cdots \\ \sqrt{1} & 0 & -\sqrt{2} & \cdots \\ 0 & \sqrt{2} & 0 & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix} \tag{18}$$

The Hamiltonian for the Harmonic, anharmonic oscillator problems can discover by utilizing the position and momentum operators.

Harmonic Oscillator

The harmonic oscillator is very useful in particle physics and is given by a ladder of evenly spaced energy levels. ΔE is the energy difference between two successive levels of the harmonic oscillator and the number of energy levels are endless. Nevertheless, there must be existent a minimum energy, since the energy must always be positive. Then, the simple harmonic oscillator Hamiltonian is

$$H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2 \tag{19}$$

where x , p , m and ω are the position, momentum, mass and angular frequency (David, C. W., 2006). The position x and momentum p can satisfy commutation relation $[x, p] = i\hbar$. In this research, natural units for mass m, angular frequency ω and $\hbar$ are used i.e. $m = \omega = \hbar = 1$. So, the reduced Hamiltonian is $H = \frac{p^2}{2} + \frac{x^2}{2}$. By $N = a_+ a_-$, the energy levels of the harmonic oscillator come to be

$$E_n = n + \frac{1}{2} \qquad\qquad n = 0, 1, 2, ... \tag{20}$$

and the wavefunctions are come $$\psi_n(x) = \left(2^n n! \sqrt{\pi}\right)^{-1/2} e^{-x^2/2} H_n(x) \tag{21}$$

where $H_n(x)$ is a Hermite polynomial. By utilizing the operators related both position and momentum, the Hamiltonian of the quantum harmonic oscillator is composed as:

$$\hat{H} = \frac{\hat{p}^2}{2} + \frac{\hat{x}^2}{2} \tag{22}$$

It is trivial to produce the Hamiltonian matrix of the simple harmonic oscillator, since it is diagonal, i.e.

$$\hat{E} = \frac{1}{2}\begin{pmatrix} 1 & 0 & 0 & \cdots \\ 0 & 3 & 0 & \cdots \\ 0 & 0 & 5 & \cdots \\ \cdots & \cdots & \cdots & \ddots \end{pmatrix} \tag{23}$$

which is the correct list containing the eigenvalues. For this case, the Eigen functions are easy to determine, since it is a diagonal matrix. By using Equation (21) and (23), Simple Harmonic Oscillator Potential V(x), it's the first thirteen energy levels and their wave function are demonstrated in Figure 1. From this figure, Eigen Functions have a notable property that each Eigen function is related with a certain Eigen energy value of the particle.

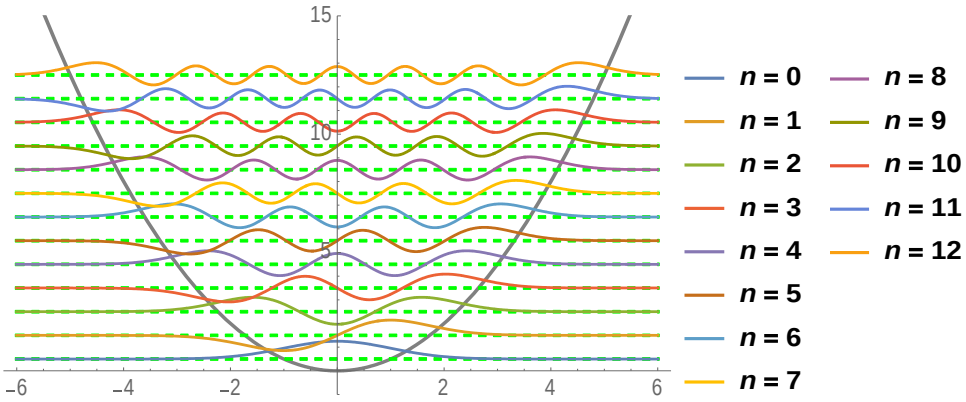

Figure 1 Simple Harmonic Oscillator Potential V(x) (Black line), the first thirteen energy levels (green dash line) and their wave function (colorful lines for each excited state)

Anharmonic Oscillator

Anharmonic oscillator, an oscillator that is not oscillating in a harmonic motion, one which diverges from the exact form of the harmonic oscillator (Pingak, R. K., Johannes, A. Z., et. al, 2021). By Equation (3), the wave function can be written in another orthonormal set form. The numerical derivation of the quartic anharmoinc oscillator is followed with the potential energy of the form

$$V(x) = ax^2 + bx^4 \tag{24}$$

In this research, the value of a is used by "0.5" for anharmonic oscillator. So, the anharmonic oscillator potential becomes

$$V(x)=\frac{x^2}{2}+bx \ ,$$

and Hamiltonian develops $$H=H_0+bH' \tag{25}$$

Applying the matrix method, the Hamiltonian Matrix's elements can be obtained by the standard method, i.e., $$H_{mn}=\langle m|H_0|n\rangle+b\langle m|x|n\rangle \tag{26}$$

The first term is the famous matrix element of unperturbed harmonic oscillation and the second term can be easily calculated using Equation (15). Once the Hamiltonian matrix elements of the an-harmonic oscillators shown above Equation (26) are calculated for a particular matrix size *N* with particular values of coupling constants to obtain *N* energy eigenvalues of the oscillators, which was completed using a athematica code in this research (Lucha, W., 1999):

$$H=\begin{pmatrix} \frac{1}{2}+\frac{3b}{4} & 0 & \frac{3b}{\sqrt{2}} & \cdots \\ 0 & \frac{3}{2}+\frac{15b}{4} & 0 & \cdots \\ \frac{3b}{\sqrt{2}} & 0 & \frac{5}{2}+\frac{27b}{4} & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix} \tag{27}$$

This diagonalizing Equation (27) resulted in *N* energy eigenvalues of the systems. When matrix of *H* is infinite, Eigen values will be given by an infinite number of. Practically, the functional basis used to construct matrices. So that, only *N* lowest basis Eigen functions of $\hat{H}_0$ are used and the rank of matrices is *N*+1. If one is especially using numerical methods, but in this case, solving energy levels using a computer program becomes easier. Now the first ten energies of the anharmonic oscillator (*b* = 0.2) for different basis states are shown in Table 1. From Table1 it obviously shows that increasing the number of basis states does have a major effect on the accuracy of the energies obtained. This result outcome comes to be more substantial as one goes to higher order anharmonicities. So, it was found that for much larger basis size, this has a more significant effect. The wave function with different basis size for energy level 8 and 9 are demonstrated by Figure 2 and 3. This figures clearly show that the wave functions are become more and more accurate by increasing the basis size *N*. Then, the potential, Eigen values and Eigen functions for the anharmonic oscillator are shown in Figure 4 as a single plot.

Table 1 The Eigen values of anharmonic oscillator at different levels *n* for different matrix dimension size *N*

n	N=20	N=50	N=100	N=200
0	0.6024051508367525	0.6024051636862472	0.6024051636862515	0.6024051636862132
1	1.9505434140535436	1.950543525634791	1.9505435256347778	1.950543525634835
2	3.5363012292982625	3.5362993632354374	3.5362993632354596	3.536299363235454
3	5.291301898243534	5.29126854258967	5.291268542589542	5.291268542589492
4	7.184415333986799	7.184456293014251	7.184456293009916	7.184456293009918
5	9.194411698495397	9.196339507067782	9.196339507035822	9.19339507035853
6	11.31115495393114	11.313238526270586	11.313238526463659	11.313238526463644

n	N=20	N=50	N=100	N=200
7	13.57964103048524	13.524907023498818	13.524907026874905	13.524907026874862
8	15.708586913924984	15.823319026413065	15.823319030455622	15.823319030455627
9	17.767683505805834	18.201980751867296	18.201980586487824	18.20198058648763
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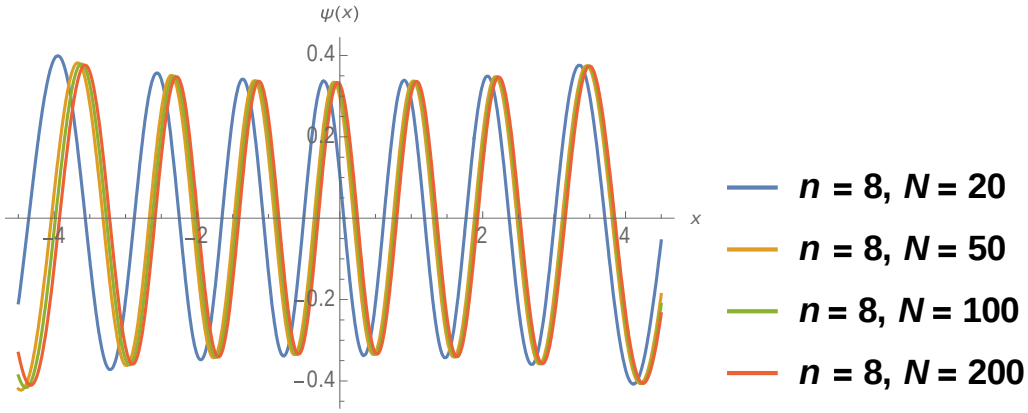

Figure 2 The wave functions of the anharmonic oscillator for energy level 8 with difference matrix dimension size *N*

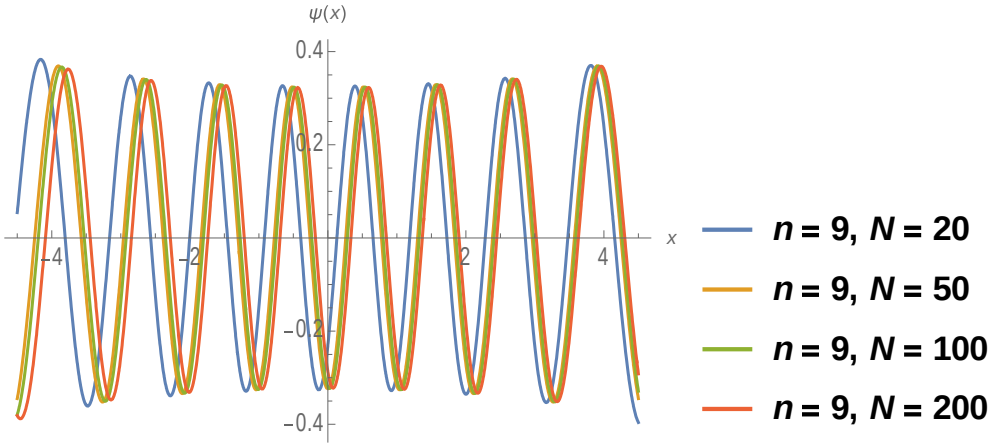

Figure 3 The wave functions of the anharmonic oscillator for energy level 9 with difference matrix dimension size *N*

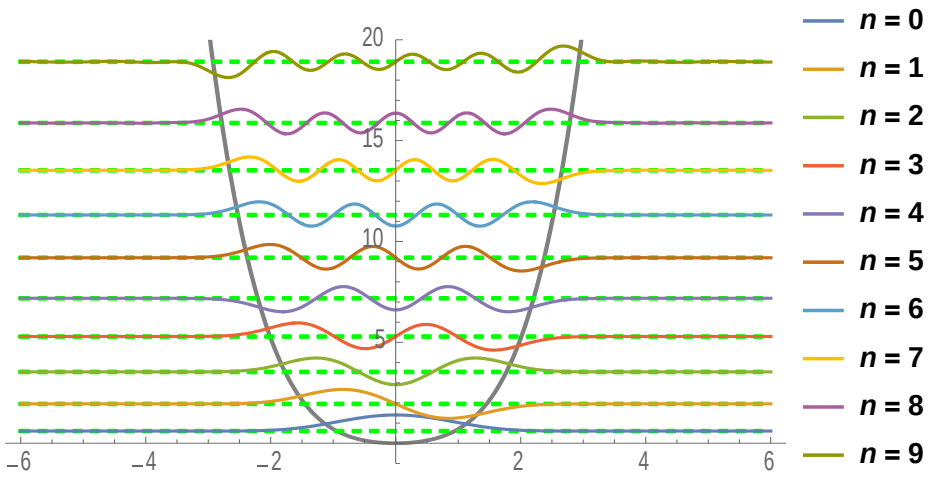

Figure 3 Anharmonic Oscillator Potential V(*x*) (Black line), the first ten energy levels (green dash line) and their wave function (colorful lines)

Conclusion

The aim of this research was to formulate a matrix method for solving the Schrödinger equation. So, the Hamiltonian matrix directly as done for the harmonic Hamiltonian equation was derived. In this step, a remarkable property has been found that each Eigen function is linked with particular Eigen energy value of the particle. According to the results of anharmonic oscillator, one can conclude that increasing the number of basis states have a major effect on the accuracy of the energies and wavefunctions. Besides, the energy values are bit by bit approching to the exact values by increasing in the number of decimal places. In this research paper, all Eigen values and Eigen functions are obtained by a result of a single computation. This is the advantage of matrix formalism. Since the matrix method can reproduce the Eigen values and its corresponding wave functions, this method is successfully modelled for the harmonic and anharmonic oscillator. Finally, this research had an adequate amount of results to make a concrete conclusion that the matrix method actually solves the Schrödinger equation, and it has a wide range of applications where it can be applied such as quantum tunneling to study a particle moving in a region of more than one constant potential or helping quantum mechanics students study solutions for anharmonic oscillators and so forth.

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