New Solution for Quantum Harmonic Oscillator Hamiltonian based on the Recurrence Formula and Jacobi matrix methods

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Abstract. Quantum Harmonic oscillator is one of the most important and beautiful models in physics. Oscillations are found throughout nature, in such things as electromagnetic waves, vibrating molecules, and the gentle back-and-forth sway of a tree branch. Quantum harmonic oscillator is used to introduce The Recurrence Formula and Jacobi matrix concept easily. Solution for Harmonic Oscillator model Hamiltonian are obtained by using the Recurrence Formula and Jacobi matrix. There isn't any restriction on the parameters.

Keywords: Quantum Harmonic oscillator, The Recurrence Formula, Jacobi matrix

Introduction

Harmonic oscillator has important role in physics. Physicists always use it for initial concepts. It can model the bond in a molecule as a spring connecting two atoms and use the harmonic oscillator expression to describe the potential energy for the periodic vibration of the atoms. The isotropic three-dimensional harmonic oscillator potential allows analytical solutions. It comprises one of the most important examples of elementary Quantum Mechanics. There are several reasons for its pivotal role. The linear harmonic oscillator describes vibrations in molecules and their counterparts in solids, the phonons. Many more physical systems can, at least approximately, be described in terms of linear harmonic oscillator models. However, the most eminent role of this oscillator is its linkage to the boson, one of the conceptual building blocks of microscopic physics. For example, bosons describe the modes of the electromagnetic field, providing the basis for its quantization. The linear harmonic oscillator, even though it may represent rather non-elementary objects like a solid and a molecule, provides a window into the most elementary structure of the Physical world. The most likely reason for this connection with fundamental properties of matter is that the harmonic oscillator Hamiltonian is symmetric in momentum and position, both operators appearing as quadratic terms. Every single book on quantum mechanics gives the solution of the harmonic oscillator problem. The reasons for that are, at least, two: (i) it is a simple problem, amenable to different methods of solution, such as the Frobenius method for solving differential equations [1, 2], and the algebraic method leading to the introduction of creation and annihilation operators [3]. This problem has therefore a natural pedagogical value; (ii)the system itself has immense applications in different fields of physics and chemistry[4, 5] and it will appear time and time again in the scientific life of a physicist There are mainly two mathematical descriptions of the quantum harmonic oscillator: (1) the direct “brute force” solution of the Schrödinger differential equation and (2) through the more elegant but more abstract ladder operators.

This section provides an in-depth discussion of a basic quantum system. The case to be analyzed is a particle that is constrained by some kind of forces to remain at approximately the same position. This can describe systems such as an atom in a solid or in a molecule. If the forces pushing the particle back to its nominal position are proportional to the distance that the particle moves away from it, you have what is called a harmonic oscillator. Even if the forces vary nonlinearly with position, they can often still be approximated to vary linearly as long as the distances from the nominal position remain small .There is traditional testing ground for new approximation techniques, that is numerically solvable.[6,7] And there are different methods for solving Hamiltonian similar as Beth-ansatz, QRPA,RPA, Hartree-Fock [8,9,10] In this paper we overview Harmonic oscillator model then Based on the recursion relation formulas and the Jacobi matrix from the theory of orthogonal polynomials, a numeric solution for these Hamiltonian model is given, without considering any restriction on the parameters specifying the strengths of the interactions.

Spectrum distribution, Recurrence Formula and Jacobin matrix Formula

We suppose unit vector $|\phi_n\rangle$ with the following representations.

$$|\phi_i\rangle = \begin{cases} |J, J-2k_i\rangle & \text{for } k_i = 0,1,...,J \\ |J, J-(2k_i+1)\rangle & \text{for } k_i = 0,1,...,J-1 \end{cases} \qquad (2\text{-}1)$$

We act the Hamiltonian H on these unit vectors and find the coefficients according to this relation [11]

$$H|\phi_i\rangle = \beta_{i+1}|\phi_{i+1}\rangle + \alpha_i|\phi_i\rangle + \beta_i|\phi_{i-1}\rangle \qquad i = 0,1,...,n \qquad (2\text{-}2)$$

As we have in ref.[11]

$$x\begin{pmatrix} Q_0(x) \\ Q_1(x) \\ Q_2(x) \\ . \\ . \\ . \\ . \\ Q_{n-1}(x) \end{pmatrix} = \begin{pmatrix} \alpha_0 & \beta_0 & 0 & 0 & . & . & . & 0 \\ \beta_0 & \alpha_1 & \beta_1 & 0 & . & . & . & 0 \\ 0 & \beta_1 & \alpha_2 & \beta_2 & . & . & . & 0 \\ . & . & . & . & & & & 0 \\ . & . & . & . & & & & . \\ . & . & . & . & & & & . \\ . & . & . & . & & & & . \\ 0 & 0 & 0 & 0 & . & . & . & \alpha_{N-1} \end{pmatrix} \begin{pmatrix} Q_0(x) \\ Q_1(x) \\ Q_2(x) \\ . \\ . \\ . \\ . \\ Q_{N-1}(x) \end{pmatrix} + \begin{pmatrix} 0 \\ 0 \\ 0 \\ . \\ . \\ . \\ 0 \\ \beta_{n-1}Q_N(x) \end{pmatrix}$$

(2-3)

If X be a zero of $Q_N(x)$,say x= x_i then we obtain $X_iQ(X_i) = JQ(X_i)$ where J is called Jacobi matrix[11] and the eigenvalues $x_1,...,x_N$ of that are the zeros of $Q_n(x)$and the eigenvector corresponding to $x_i$is $Q_0(x_i),Q_1(x_i),...,Q_{N-1}(x_i)$.If we choose x= $x_i$then the end matrix will be zero, therefore the coefficients α and β are equal to the coefficients in the recursion relations.

$$Q_0(x) = 1, \qquad Q_1(x) = x - \alpha_1$$

$$xQ_k(x) = Q_{k+1}(x) + \alpha_{k+1}Q_k(x) + \beta_k^2 Q_{k-1}(x), \quad k \geq 1. \qquad (2\text{-}4)$$

Harmonic oscillator

Quantum harmonic oscillator involves square law potential in the Schrodinger equation and is a fundamental problem in quantum mechanics. For investigation of Recursion Formula and Jacobi Matrix we will consider simple Harmonic oscillator. At first We will solve it analytically then compare with this method.cosider a vertical spring with hardship coefficient K that a body with mass m hanging it(as figure 1) . Total force obtained when weight (mg) added to it and Hamiltonian written as below:

$$H = \frac{P^2}{2m} + \frac{1}{2}mw^2x^2 - mgx \qquad (3\text{-}5)$$

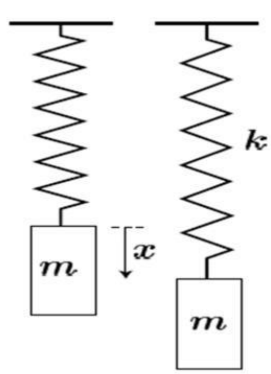

Figure 1

$$mw^2x - mg = 0 \qquad (3\text{-}6)$$

$$x_0 = \frac{g}{w^2} \quad (3\text{-}7)$$

Then we will define new coefficient as

$$X = x - \frac{g}{w^2} \qquad (3\text{-}8)$$

Hamiltonian written with new confidents is

$$H = \frac{P^2}{2m} + \frac{1}{2}mw^2\left(x - \frac{g}{w^2}\right)^2 - \frac{1}{2}mw^2\left(\frac{g^2}{w^4}\right) \quad (3\text{-}9)$$

Then new Energy spectrum by old spectrum is written as:

$$E_f = E_i - \frac{1}{2}m\frac{g^2}{w^2} \quad (3\text{-}10)$$

The Hamiltonian of the Harmonic oscillator model can be written as:

$$H = \hbar w\left(a^\dagger a + \frac{1}{2}\right) - mg\sqrt{\frac{\hbar}{2mw}}(a + a^\dagger) \quad (3\text{-}11)$$

We will choice unit vector as

$$\left|\psi_n\right\rangle = \frac{a^{\dagger n}}{\sqrt{n!}}\left|0\right\rangle \qquad (3\text{-}12)$$

After effecting Hamiltonian on it we have

$$a^\dagger a\left|\psi_n\right\rangle = a^\dagger a\frac{a^{\dagger n}}{\sqrt{n!}}\left|0\right\rangle = \frac{a^\dagger a a^\dagger a^{n-1}}{\sqrt{n!}}\left|0\right\rangle = \qquad (3\text{-}13)$$

$$a^\dagger(a^\dagger a + 1)\frac{a^{\dagger n-1}}{\sqrt{n!}}\left|0\right\rangle = \frac{a^{\dagger 2} a a^{\dagger n-1}}{\sqrt{n!}}\left|0\right\rangle + \frac{a^{\dagger n}}{\sqrt{n!}}\left|0\right\rangle = \left|\Psi_n\right\rangle + \frac{a^{\dagger 2} a a^\dagger a^{\dagger n-2}}{\sqrt{n!}}\left|0\right\rangle \quad (3\text{-}14)$$

$$= \left|\Psi_n\right\rangle + \frac{a^{\dagger 2}(a^\dagger a + 1)a^{\dagger n-2}}{\sqrt{n!}}\left|0\right\rangle = 2\left|\Psi_n\right\rangle + \frac{a^{\dagger 3} a a^{\dagger n-2}}{\sqrt{n!}}\left|0\right\rangle$$

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. (3-15)

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$$= n\left|\Psi_n\right\rangle$$

the first Hamiltonian section written by numeric operator will be:

$$\hbar w\left(a^\dagger a + \frac{1}{2}\right) = \hbar w\left(n + \frac{1}{2}\right) \qquad (3\text{-}16)$$

Considering the other sentences and effecting $\left|\Psi_n\right\rangle$ on them

$$a\left|\psi_n\right\rangle = a\frac{a^{\dagger n}}{\sqrt{n!}}\left|0\right\rangle = \qquad (a^\dagger a + 1)\frac{a^{\dagger n-1}}{\sqrt{n!}}\left|0\right\rangle = \frac{a^\dagger a a^{\dagger n-1}}{\sqrt{n!}}\left|0\right\rangle + \frac{a^{\dagger n-1}}{\sqrt{n(n-1)!}}\left|0\right\rangle$$

$$= a^\dagger (a^\dagger a + 1) \frac{a^{\dagger n-2}}{\sqrt{\mathrm{n}!}} |0\rangle + \frac{1}{\sqrt{n}} |\psi_{n-1}\rangle = \frac{a^{\dagger 2} a a^{\dagger n-2}}{\sqrt{n!}} |0\rangle + \frac{2}{\sqrt{n}} |\psi_{n-1}\rangle$$

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$$= \frac{n}{\sqrt{n}} |\Psi_{n-1}\rangle = \sqrt{n} |\Psi_{n-1}\rangle$$

(3-17)

$$a^\dagger |\psi_n\rangle = a^\dagger \frac{a^{n\dagger}}{\sqrt{\mathrm{n}!}} |0\rangle = \frac{a^{\dagger \mathrm{n}+1}}{\sqrt{\mathrm{n}!}} |0\rangle = \sqrt{n+1} |\psi_{n+1}\rangle \quad (3\text{-}18)$$

Then from collecting the above results we will have:

$$H|\psi_n\rangle = \hbar w(n + \frac{1}{2})|\psi_n\rangle - mg\sqrt{\frac{n\hbar}{2mw}}|\psi_{n-1}\rangle - mg\sqrt{\frac{(n+1)\hbar}{2mw}}|\psi_{n+1}\rangle \quad (3\text{-}19)$$

from comparing the upper relations with recurrence formula we will distinguish the $\alpha_n$and β_n as:

$\alpha_n = \hbar w \left(n + \frac{1}{2}\right) \qquad \beta_n = mg\sqrt{\frac{n\hbar}{2mw}}$ (3-20)

With supposing coefficients as

$w = 10 \qquad m = 1 \qquad \hbar = 1$

so we will have:

$\alpha_1 = \frac{3}{2}\hbar w = 15$ (3-21)

$\alpha_2 = \hbar w \left(2 + \frac{1}{2}\right) = 25$ (3-22)

$\beta_1 = \sqrt{1} \times 1 \times g \times \sqrt{\frac{1}{2\times1\times10}} = \frac{g}{\sqrt{20}} = 0.223g$ (3-23)

$\beta_2 = \sqrt{2} \times 1 \times g \times \sqrt{\frac{1}{2\times1\times10}} = g \times \sqrt{\frac{2}{20}} = 0.316g$ (3-24)

For example the first three recursion sentence will be:

$q_0 = 1 \quad q_1 = x - \alpha_1 = x - 15$ (3-25)

$q_2 = (x - \alpha_2)q_1 = (x - 25)(x - 15) + 0.223g^2$ (3-26)

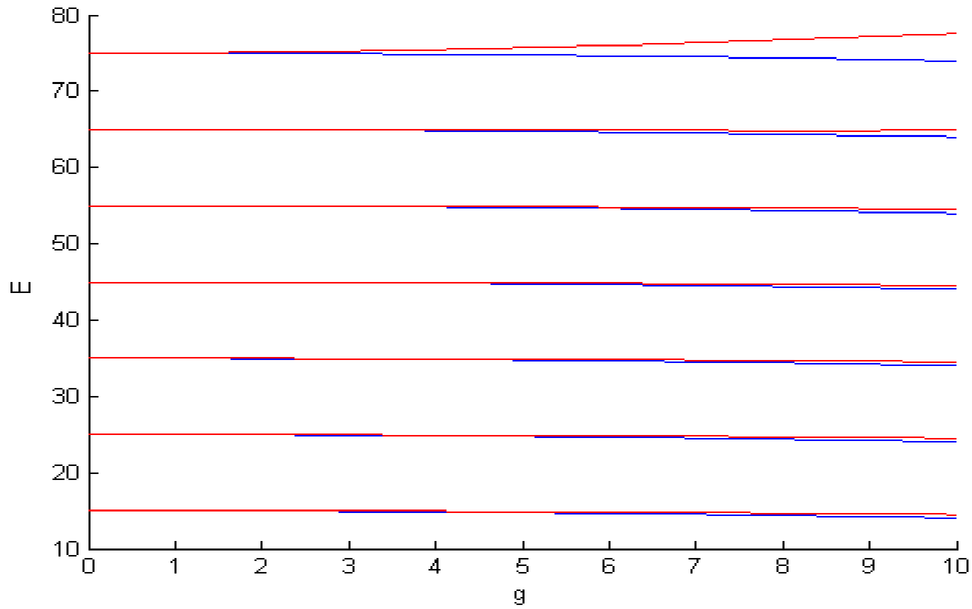

Figure 2. Comparing analytical method (blue color) with numerical method (red color)

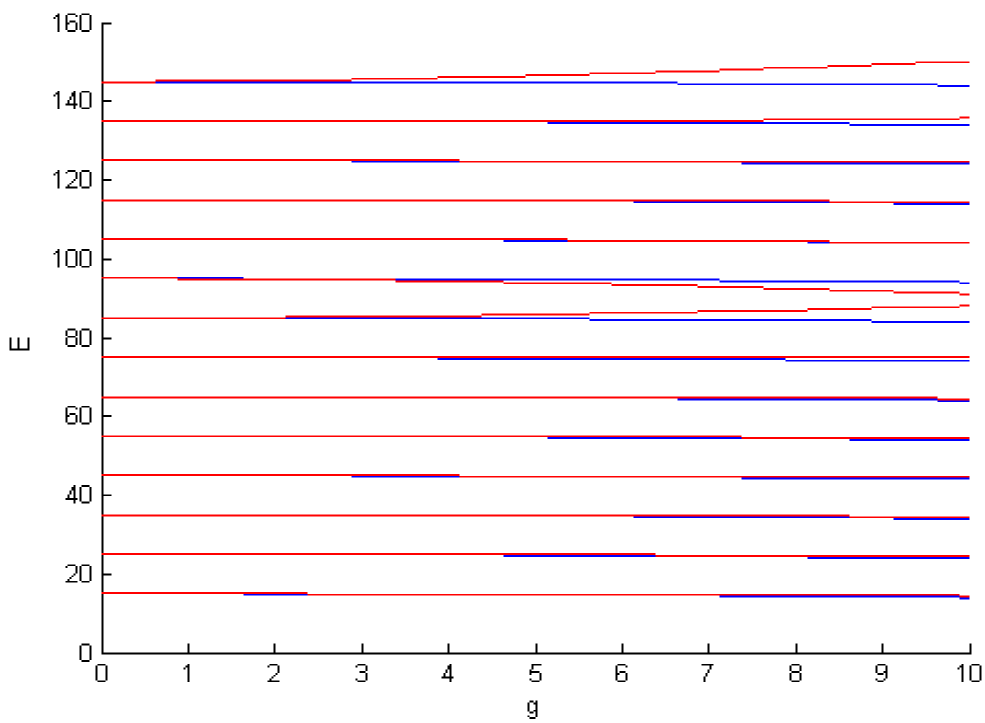

Figure 3. Comparing analytical method (blue color) with numerical method (red color)}.

Conclusions and Discussions

In this article we got solution for the Harmonic Oscillator model. It can be solved by various conventional methods such as (i) analytical methods where Hermit polynomials are involved, (ii) algebraic methods where ladder operators are involved, and (iii) approximation methods where perturbation, variational, semiclassical, etc. techniques are involved. We got solution by using the Recurrence Formula and Jacobi matrix. In Harmonic Oscillator graphs, we compare analytical method with numerical method. Clearly shows that these method have the same conclusions.

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