

ORIGINAL RESEARCH ARTICLE

Approximate Solution of Schrodinger Equation to Diatomic Molecule for Harmonic Oscillator

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ABSTRACT

This study has described the approximate solution of Schrodinger equation to diatomic molecule for harmonic oscillator. The solution procedure is developed by the Power series method and Newton's second law. It consider an approximate solution of harmonic oscillator using Schrödinger equation in one dimension only because other analytical approaches are limited to the widely known method and consider two to five dimensions with various iteration method to obtain their results but here the solutions to be obtained and their efficiency will help other research to comprehend how the solution of this harmonic oscillator has been done over the years and also to use the most efficient approximate solution.



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INTRODUCTION

The brand new paradigm in physics, which emerged at the beginning of the final century and is now commonly called Schrodinger equation that describes the wave function of a quantum mechanical machine changed into stimulated by two sorts of experimental observations Planck could effectively calculate the spectrum of black-frame radiation in 1900 via postulating that an electromagnetic field can change electricity with atoms only in quanta which can be the made from the radiation frequency and the famous constant, which become later named after him (David and Sabine, 2006). While for Planck himself, the introduction of his constant turned into an act of desperation, entirely justified via the settlement of the calculated with the measured spectrum, Albert Einstein took the idea critical. In his clarification of the photoelectric impact in 1905, he considered light itself as composed of particles carrying a discrete energy. This formidable view became in blatant contradiction with the through then installed belief of mild as an electromagnetic wave. Newton's 2nd law reads, the net pressure performing on a body is same to the overall time by-product of the whole momentum of that body was used to make a mathematical prediction as to what path a given bodily machine would take through the years following a hard and fast of recognized initial

conditions. Fixing this equation offers the physical gadget's position and momentum as a feature of the outside pressure at the machine. Those two parameters are enough to explain its country at on every occasion on the spot.

In quantum mechanics, the analogue of Newton's regulation is Schrödinger's equation (Schrödinger, 1926). The Schrödinger equation is a linear partial differential equation (PDE) that describes the wave characteristic of a quantum-mechanical system (David, 2004). It is a key to bringing about quantum mechanics, and its discovery become a sizeable landmark in developing the concern. The equation is named after Erwin Schrödinger, who postulated the equation in 1925, and posted it in 1926, forming the basis for the paintings that resulted in his nobel prize in Physics in 1933. Several studies have been conducted on Schrodinger equation. Akaninyeye, Christian and Louis (2019) studied the Schrodinger equation in the cylindrical basis with a harmonic oscillator using a Nikiforov-Uvarov method. The energy eigenvalues and the normalized wave characteristic in cylindrical basis ρ, ϕ, z in the form

$$V(\rho, z) = \frac{\omega^2}{2} (z^2 + \rho^2) \text{ where } \omega \text{ is the frequency}$$

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of the oscillator obtained, Which suggests that the oscillator propagated along the axis of symmetry of harmonic oscillator potential. [Harko and Liang \(2018\)](#) investigated the connection between the linear harmonic oscillator equation and a few lessons of second order non-linear ordinary differential equations of generalized lienard type, which physically describe crucial oscillator structures the usage of a way in quantum mechanics that incorporate the deformation of the segment area coordinate of the harmonic oscillator. They generalized the equation of motion of the classical linear harmonic oscillator to several training of intensely non-linear differential equations. The devised technique may be similarly generalized to derive explicit widespread solution of non-linear second order differential equation unrelated to the harmonic oscillator. The real existence applications of the acquired results are used for the touring wave answer of the reaction-convection-diffusion equations and the huge amplitude loose vibrations of a uniform cantilever beam. [Bonilla and Rosas \(2017\)](#) investigated the harmonic oscillator within the framework of scale fantastically where the dynamic regulation obeyed with the aid of the only-dimensional physical structures inside the scale extraordinarily technique which reduced to a Riccati non-linear differential

$$W = \frac{m}{2} \vec{v}^2 + \Phi - i \frac{\hbar}{2} (\vec{\nabla} \cdot \vec{v})$$

equation.

Riccati nonlinear differential equation is implemented to the harmonic oscillator potential, which ends up to the calculation of the answers of the scale exceptionally problem in phrases of the well-known solution of the Schrödinger equation for the harmonic oscillator.

Several studies have been conducted on Schrodinger equation. [Alharbey, et.al \(2019\)](#) investigated chirped Gaussian pulse excitation of a harmonic oscillator and stated the basic problem of the interplay of a single quantized mode of the radiation field, modelled as quantized harmonic oscillator with a laser pulse of chirped Gaussian line-shape. The average photo wide variety and the brief emitted spectrum are calculated analytically in phrases of the error feature of complicated argument. The spectral peaks of the line shape of the emitted radiation are tested for exclusive system parameters and preliminary states of the harmonic oscillator. [Richard \(2018\)](#) worked on solutions of the fractional Schrödinger equation via diagonalization - a plea for the harmonic oscillator basis. A covariant non-neighbourhood extension of the desk bound Schrödinger equation was provided and its solution in terms of Heisenberg's matrix

quantum mechanics became proposed. For the special case of the Riesz fractional derivative, the calculation of corresponding matrix factors for the non-local kinetic energy term turned was carried out completely analytically inside the harmonic oscillator foundation and led to a new interpretation of non-nearby operators in terms of generalized Glauber states. As a first application, the capability power matrix factors are calculated for the fractional harmonic oscillator and the corresponding Schrödinger equation become diagonalized. For the special case of invariance of the non-nearby wave equation under Fourier-transforms, a new symmetry became deduced, which can be interpreted as an extension of the standard parity-symmetry. [Lawson, Gabriel and Laure \(2018\)](#) studied Lewis-Riesenfeld quantization and SU (1,1) coherent states for 2D damped harmonic oscillator where in the classical level, they solved the equations of motion for a specific case of the time-dependent coefficient of friction and at the quantum level, they used the Lewis-Riesenfeld technique of invariants to construct exact solutions for the corresponding time-based Schrodinger equations. The eigenfeatures obtained are in phrases of the generalized Laguerre polynomials solutions which result in generalization version of Heisenberg's uncertainty relation and the generators of the su(1,1) lie algebra. [Chang \(2019\)](#) studied responses to frequency modulation in a quantum harmonic oscillator and considered the frequency modulation reaction in terms of the time dependence of quasi energies and the deviation from the quantum virial theorem. Four modulation kinds are considered: linear, quadratic, exponential, and sinusoidal. [Alakesh et al. \(2019\)](#) worked on an experimental demonstration of force driven quantum harmonic oscillator in an IBM quantum computer and tested a quantum simulation of QHO within the presence of both time-varying and constant force field for each one and dimensional case. New quantum circuits are advanced to simulate each the one and two-dimensional QHO and are applied at the real quantum chip "ibmqx4". Experimental information, really illustrating the dynamics of QHO in the presence of time-established force field, is presented in graphs for exclusive frequency parameters within the Hamiltonian picture and quantum simulation of many bodily structures can be understood from the simulation of the quantum harmonic oscillator.

In the past other methods have been used to solve the harmonic oscillator including Dirac Equation, Nikiforov-Uvarov method, perturbation theory, vibrational method and shooting method. Use of Schrodinger's equation in solving the harmonic

METHOD OF SOLUTION FOR HARMONIC OSCILLATOR

oscillator have been on the rise, power series and Newton’s second law are incorporated with Schrodinger so as to converge to a solution faster and give an accurate error free solution. Thus, there has been a need to obtain approximate solution of one-dimension problem to harmonic oscillator by testing the result accuracy which in this study using Schrodinger’s equation method.

Here we present the technique utilized in organising the approach to the Schrödinger equation for the harmonic oscillator. We consider the figure below, which describes the vibration of a diatomic molecule *HCL*, to be a one-dimensional problem in that the two atoms only move toward or away from one another in a single direction *x*.

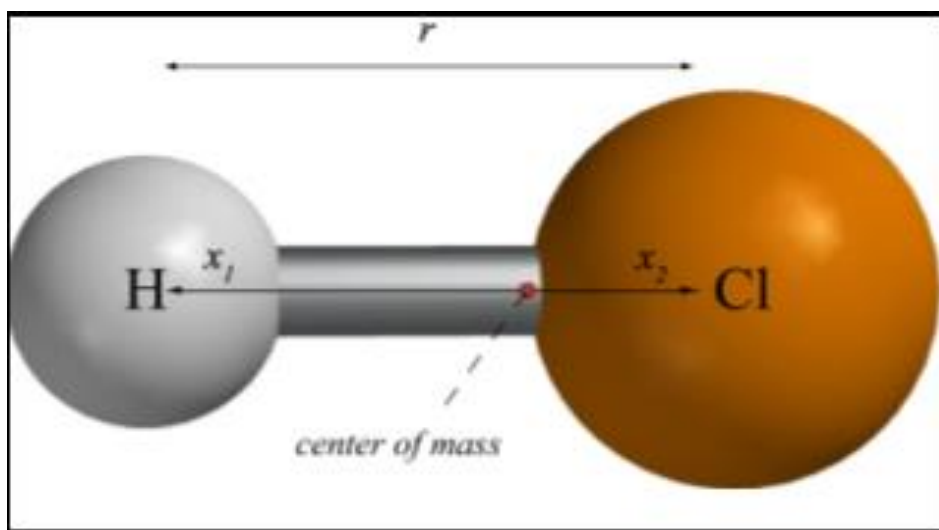


Figure 1: Vibration of diatomic molecule (HCL)

Using Figure 1, we let x_1 be the position of the hydrogen atom from the centre of mass of the molecule and also let x_2 the position of the chlorine from the centre of mass of the molecule. The separation between the atoms is defined as $r = x_2 - x_1$ and

$$x_1 = \frac{m_2}{m_1 + m_2} r \text{ and } x_2 = \frac{m_1}{m_1 + m_2} r \tag{1}$$

During harmonic vibration, the atoms oscillate about an equilibrium separation, r_e , where we can define x as the deviation from that equilibrium separation, i.e., $x = r - r_e$. The motion is constrained by a force that, to a good approximation, is proportional to the deviation from equilibrium, x , and operates in the opposite direction to the motion, i.e., a restoring force, such that

$$\vec{F} = -k\vec{x} \quad (\text{Hooke's law}) \tag{2}$$

The proportionality of constant, k , is called the force constant.

The nature of the oscillating motion can be realized by equating force to mass times acceleration for each atom,

$$\vec{f}_1 = m_1 \vec{a} = m_1 \frac{d^2 x_1}{dt^2} = -k\vec{x} \quad \text{and} \tag{3}$$

$$\vec{f}_2 = m_2 \vec{a} = m_2 \frac{d^2 x_2}{dt^2} = -k\vec{x}$$

Replacing x_1 and x_2 in (2) from (3) for both f_1 and f_2 , we find

$$\vec{f} = \frac{m_1 m_2}{m_1 + m_2} \frac{d^2 r}{dt^2} = -k\vec{x} \tag{4}$$

Recognizing $\frac{m_1 m_2}{m_1 + m_2}$ as the reduced mass, μ , and $\vec{r} = \vec{x} + \vec{r}_e$, where \vec{r}_e is a constant; (4) becomes

$$\vec{f} = \mu \frac{d^2 \vec{x}}{dt^2} = -k \vec{x} \tag{5}$$

Thus, the problem of an oscillating diatomic is reduced to the departure of a single mass, μ , from its equilibrium separation from a fixed reference, r_e .

The solution to (5) yields \vec{x} as a sinusoidal function of t

$$\vec{x} = A \sin \left[\left(\frac{k}{\mu} \right)^{\frac{1}{2}} t + b \right] \tag{6}$$

where b is a phase constant and $\left(\frac{k}{\mu} \right)^{\frac{1}{2}}$ has units of

reciprocal time or frequency, $\omega = 2\pi\nu$

Conservation of energy requires that any work done moving the reduced mass against the restoring force, $\delta\omega = \vec{f}d\vec{x}$, must be countered an opposing change in the potential energy.

$$\delta\omega = \vec{f}d\vec{x} = -dV(x) \tag{7}$$

or

$$\vec{f} = -k\vec{x} = -\frac{dV(x)}{d\vec{x}} \tag{8}$$

Integrating (8), we find the functional dependence of $V(x)$ on x

$$V(x) = \frac{1}{2} kx^2 + C \tag{9}$$

where C is a constant of integration.

SCHRODINGER EQUATION

We can apply this potential energy in (9) to the Schrödinger equation, to find any quantization of energies of the harmonic oscillator. Doing so, while replacing m with the reduced mass, μ , yields

$$-\frac{\hbar^2}{2\mu} \frac{\partial^2}{\partial x^2} \psi_n(x,t) - \frac{1}{2} kx^2 \psi_n(x,t) = E_n \psi_n(x,t) \tag{10}$$

Rearranging (10)

$$\frac{\partial^2}{\partial x^2} \psi_n(x,t) - \frac{\mu k x^2}{\hbar^2} \psi_n(x,t) + \frac{\mu E_n}{\hbar^2} \psi_n(x,t) = 0 \tag{11}$$

simplifying by letting $\alpha^2 = \frac{\mu k}{\hbar^2}$, such that the Schrödinger equation becomes

$$\frac{\partial^2}{\partial x^2} \psi_n(x,t) + \left[\frac{2\mu E_n}{\hbar^2} - \alpha^2 x^2 \right] \psi_n(x,t) = 0 \tag{12}$$

To obtain the basis set, $\{\psi_n(x,t)\}$, that satisfies this equation by first considering the asymptotic solution at large x . At large $x, \alpha^2 x^2 \gg \frac{2\mu E_n}{\hbar^2}$, and (12) collapses to

$$\frac{\partial^2}{\partial x^2} \psi_n(x,t) - \alpha^2 x^2 \psi_n(x,t) = 0$$

The solution to (13) are Gaussian, Hence $\psi_n(x,t) = e^{\pm\alpha x^2/2} e^{-i\omega_n t}$

But only $e^{-\alpha x^2/2}$ satisfies the global constraint of quadratic integrality, with $e^{+\alpha x^2/2}$ grows largely as $x \rightarrow \infty$

The general form of solution at all x ,

$$\psi_n(x,t) = f_n(x) e^{\pm\alpha x^2/2} e^{-i\omega_n t}$$

where $f_n(x)$ represent the shape of the wave function because of the time-dependent part of the wave function, $T(t)$ in $\psi_n(x,t) = \psi(x)T(t)$, slides through the spatial operators in (12), we can simplify the process of finding $f_n(x)$ by first ignoring $T(t)$.

Applying the spatial part of our trial basic set of function $\psi_n(x) = f_n(x) e^{-\alpha x^2/2}$ to (12).

Beginning with the first derivative of $\psi_n(x)$, we find

$$\frac{\partial}{\partial x} \psi_n(x) = f_n(x) (-\alpha x) e^{-\alpha x^2/2} + e^{-\alpha x^2/2} \frac{d}{dx} f_n(x) \tag{15}$$

The second derivative is then

$$\frac{\partial^2}{\partial x^2} \psi_n(x) = \left[f_n(x)(-\alpha x) + \frac{d}{dx} f_n(x) \right] (-\alpha x) e^{-\alpha x^2/2} + e^{-\alpha x^2/2} \left[f_n(x)(-\alpha) - \alpha x \frac{d}{dx} f_n(x) + \frac{d^2}{dx^2} f_n(x) \right] \quad (16)$$

Or simplifying

$$\frac{\partial^2}{\partial x^2} \psi_n(x) = e^{-\alpha x^2/2} \left[f_n(x)(\alpha^2 x^2) - \alpha f_n(x) - 2\alpha x \frac{\partial}{\partial x} f_n(x) + \frac{\partial^2}{\partial x^2} f_n(x) \right] \quad (17)$$

Completing (12); (18) cancelling the term in $(\alpha^2 x^2)$

and requiring the coefficient of $e^{-\alpha x^2/2}$ to sum to zero, because no such term survives on the right side, we find an equation in $f_n(x)$

$$\frac{\partial^2}{\partial x^2} f_n(x) - 2\alpha x \frac{\partial}{\partial x} f_n(x) - \alpha f_n(x) + \frac{2\mu E_n}{h^2} f_n(x) = 0 \quad (19)$$

APPLICATION OF POWER SERIES TO SCHRÖDINGER EQUATION

Having established (19) above, it is therefore considered here that power series can be applied to Schrödinger equation. However, since we know little about the nature of $f_n(x)$, we apply a general utility power series.

$$f_n(x) = \sum_{n=0}^{\infty} C_n X^n = C_0 + C_1 x + C_2 x^2 + C_3 x^3 + \dots \quad (20)$$

Differentiating (20) again in a stepwise fashion

$$\frac{\partial}{\partial x} f_n(x) = \sum_{n=1}^{\infty} n C_n X^{n-1} = \sum_{n=0}^{\infty} n C_n X^{n-1} = C_1 + 2C_2 x + 3C_3 x^2 + \dots \quad (21)$$

Applying $f_n(x)$ again in a stepwise fashion to (19) with the second summation running from $n=0$, because that term is zero.

The second derivative then becomes

$$\frac{\partial^2}{\partial x^2} f_n(x) = \sum_{n=2}^{\infty} n(n-1) C_n X^{n-2} = \sum_{n=0}^{\infty} (n+2)(n+1) C_{n+2} X^n = 2C_2 + 6C_3 x + \dots \quad (22)$$

Plugging $f_n(x)$, its first and second derivative into (19), we find

$$\sum_{n=2}^{\infty} \left[(n+2)(n+1) C_{n+2} X^n - 2\alpha n C_n X^n - \alpha n C_n X^n + \frac{2\mu E_n}{h^2} C_n X^n \right] = 0 \quad (23)$$

Since no powers of x survive on the RHS of (23), the coefficients of X^n must sum to zero. i.e.

$$(n+2)(n+1) C_{n+2} - 2\alpha n C_n - \alpha n C_n + \frac{2\mu E_n}{h^2} C_n = 0 \quad (24)$$

Rearranging (24) yields a recursion relation where C_{n+2} is related to C_n

$$C_{n+2} = \left[\frac{2\alpha n + \alpha - \frac{2\mu E_n}{h^2}}{(n+2)(n+1)} \right] C_n \quad (25)$$

Truncating the series at a finite value of n , say $n = v$. Then the coefficients C_v is finite but coefficients C_{v+1}, C_{v+2} , and higher vanish .if C_v is finite and C_{v+2} is zero, then the coefficient of C_v in (25) must be zero, i.e.,

$$2\alpha n + \alpha - \frac{2\mu E_n}{h^2} = 0 \quad (26)$$

Rearranging with substitutions for α and k , the allowed energies for the harmonic oscillator, is

$$E_v = \frac{h^2 \alpha}{\mu} \left(v + \frac{1}{2} \right) = h \frac{\sqrt{\mu k}}{\mu} \left(v + \frac{1}{2} \right) = h \nu \left(v + \frac{1}{2} \right) \quad (27)$$

With eigenvalues at

$$E_0 = \frac{1}{2} h \nu$$

$$E_1 = \frac{3}{2} h \nu$$

$$E_2 = \frac{5}{2} h\nu, \text{ etc.}$$

The Eigen functions are;

$$\psi_n(x) = f_n(x)e^{-\alpha x^2/2} = \sum_{n=0}^v C_n X^n e^{-\alpha x^2/2} \tag{28}$$

The lowest energy wave function $\psi_0(x)$, contains no power of x in the polynomial, $f_n(x)$, and collapse to the Gaussian which is an even function of x , i.e.

$$\psi_0(x) = \psi_0(-x)$$

$$\psi_0(x) = C_0 e^{-\alpha x^2/2} \tag{29}$$

Orthogonalization of the next higher energy wave function, $\psi_1(x)$ requires removal of any component of $\psi_1(x)$ that is parallel to $\psi_0(x)$, i.e., the C_0 in

$$\psi_1(x) = \sum_{n=0}^1 C_n X^n e^{-\alpha x^2/2} = C_0 e^{-\alpha x^2/2} + C_1 e^{-\alpha x^2/2} \tag{30}$$

Must be zero, otherwise there would be a component of $\psi_0(x)$ along $\psi_1(x)$.

Thus

$$\psi_1(x) = C_1 e^{-\alpha x^2/2} \tag{31}$$

which are odd functions of x ; i.e. $\psi_1(x) = -\psi_1(-x)$

The wave function of the harmonic oscillator alternates in parity, even and odd, as the energy of the oscillator increases, with either only even or only odd powers of x in each series. The coefficients, C_n , can be found by normalizing, for example

$$\begin{aligned} \int_{-\infty}^{\infty} \psi_0(x) * \psi_0(x) dx &= \int_{-\infty}^{\infty} C_0 e^{-\alpha x^2/2} C_0 e^{-\alpha x^2/2} dx : \\ &= \int_{-\infty}^{\infty} C_0^2 e^{-\alpha x^2/2} dx = C_0^2 \sqrt{\frac{\pi}{\alpha}} = 1 \end{aligned} \tag{32}$$

yielding

$$C_0 = \left(\frac{\alpha}{\pi}\right)^{\frac{1}{4}}$$

The first four wave function for the harmonic oscillator are,

$$\psi_0(x) = \left(\frac{\alpha}{\pi}\right)^{\frac{1}{4}} e^{-\alpha x^2/2} \tag{33}$$

$$\psi_1(x) = \left(\frac{4\alpha^2}{\pi}\right)^{\frac{1}{4}} x e^{-\alpha x^2/2}$$

$$\psi_2(x) = \left(\frac{\alpha}{4\pi}\right)^{\frac{1}{4}} (2\alpha x^2 - 1) e^{-\alpha x^2/2}$$

$$\psi_3(x) = \left(\frac{\alpha^3}{9\pi}\right)^{\frac{1}{4}} (2\alpha x^3 - 3x) e^{-\alpha x^2/2}$$

Considering a calculation of the most probable position for a harmonic oscillator with wave function $\psi_0(x)$. We search for the maximum in $\psi_0(x) * \psi_0(x)$, the probability density by finding where the slope is zero.

$$\frac{\partial}{\partial x} \psi_0(x) * \psi_0(x) = \frac{\partial}{\partial x} \left[\left(\frac{\alpha}{\pi}\right)^{\frac{1}{4}} e^{-\alpha x^2/2} \right]^2 = \left(\frac{\alpha}{\pi}\right)^{\frac{1}{4}} (-2\alpha x) = 0 \tag{34}$$

The roots of (34) lies at $x = \pm\infty, 0$. The root at $x = \pm\infty$, are minima, while the root at $x = 0$ is the maximum. Thus, the most probable position for an oscillator with wave function $\psi_0(x)$ is at $x = r - r_e = 0$, or at the equilibrium separation between the nuclei and at the minimum in the potential energy.

RESULTS

This session presents the results used in establishing solution to the Schrödinger equation for harmonic oscillator. Consider figure 1 which described the vibration of a diatomic molecule of *HCL* in one-dimensional problem. It is shown that two atoms only move toward or away from one another along a

single direction x resulting to masses assigned to each atomic molecule defined above and the equilibrium separation of the two atoms r_e which acted upon by a force in opposite direction as indicated in (2).

Rearranging (8) to have

$$-k\bar{x} = -\frac{dv(x)}{d\bar{x}}$$

Next is to integrate (35),

$$\int -k\bar{x} = \int -\frac{dv(x)}{d\bar{x}}$$

$$\Rightarrow \int k\bar{x} = \int \frac{dv(x)}{d\bar{x}}$$

Therefore,

$$\int k\bar{x} = v(x) \int \frac{d}{d\bar{x}}$$

which is the potential energy, and (10) can be written as

$$-\frac{h^2}{2\mu} \frac{\partial^2}{\partial x^2} \psi_n(x,t) + \frac{1}{2} kx^2 \psi_n(x,t) - E_n \psi_n(x,t) = 0$$

$$-\frac{h^2}{2\mu} \cdot \frac{2\mu}{h^2} \frac{\partial^2}{\partial x^2} \psi_n(x,t) - \frac{1}{2} kx \cdot \frac{2\mu^2}{h^2} \psi_n(x,t) + E_n \cdot \frac{2\mu}{h^2}$$

This can further be expressed as

$$\frac{\partial^2}{\partial x^2} \psi_n(x,t) - \frac{\mu k x^2}{h^2} \psi_n(x,t) + \frac{2\mu E_n}{h^2} \psi_n(x,t) = 0$$

$$\frac{\partial^2}{\partial x^2} \psi_n(x,t) + \left[\frac{2\mu E_n}{h^2} - \frac{kx^2 \mu}{h^2} \right] \psi_n(x,t) = 0$$

Now substituting α^2 for $\frac{\mu k}{h^2}$ in (39) result to (12)

which describe the Schrodinger equation. However, the second derivation of the general form of solution obtained in (13) is given by

$$\psi_n''(x,t) = \frac{\partial^2}{\partial x^2} \psi_n(x) =$$

$$f_n(x)(-\alpha x)(-\alpha x)e^{-\alpha^2 x^2/2} + (-\alpha x)e^{-\alpha^2 x^2/2} \frac{d}{dx} f_n(x)$$

$$+ f_n(x)(-\alpha)e^{-\alpha^2 x^2/2} - e^{-\alpha^2 x^2/2} \frac{d}{dx} f_n(x)(-\alpha x) + e^{-\alpha^2 x^2/2} \frac{d^2}{dx^2} f_n(x)$$

$$\frac{\partial^2}{\partial x^2} \psi_n(x) =$$

$$e^{-\alpha x^2/2} \left[f_n(x)(\alpha^2 x^2) - \alpha f_n(x) - 2\alpha x \frac{\partial}{\partial x} f_n(x) + \frac{\partial^2}{\partial x^2} f_n(x) \right] \tag{41}$$

(26) can further be simplified as follows;

$$2\alpha v + \frac{h^2 \alpha - 2\mu E_v}{h^2} = 0 \tag{35}$$

$$\alpha h^2 (2v + 1) = 2\mu E_v$$

The quantization of energies of the harmonic oscillator can be expressed as

$$E_v = \frac{\alpha h^2 (2v + 1)}{2\mu}$$

which is simplified as

$$E_v = \frac{\alpha h^2}{\mu} \cdot \frac{(2v + 1)}{2} \tag{36}$$

Hence,

$$E_v = \frac{\alpha h^2}{\mu} \left(v + \frac{1}{2} \right)$$

$$E_v = \frac{h^2 \alpha}{\mu} \left(v + \frac{1}{2} \right) = h \frac{\sqrt{\mu k}}{\mu} \left(v + \frac{1}{2} \right) \text{ Multiplying } \left(\frac{1}{2} \right) \tag{37}$$

With the quantization of energies in (43), the eigenvalues are obtained as follows;

$$E_0 = h(v) \left(0 + \frac{1}{2} \right) \Rightarrow hv \left(\frac{1}{2} \right) = \frac{1}{2} hv \tag{38}$$

$$E_1 = h(v) \left(1 + \frac{1}{2} \right) \Rightarrow hv \left(\frac{3}{2} \right) = \frac{3}{2} hv \tag{39}$$

$$E_2 = h(v) \left(2 + \frac{1}{2} \right) \Rightarrow hv \left(\frac{5}{2} \right) = \frac{5}{2} hv \tag{40}$$

$$E_3 = h(v) \left(3 + \frac{1}{2} \right) \Rightarrow hv \left(\frac{7}{2} \right) = \frac{7}{2} hv,$$

$$v = 0, 1, 2, 3, \dots$$

The Eigen functions obtained from the general form of solution in (14) can be obtained as follows;

$$\psi_0(x) = f_0(x) e^{-\alpha x^2/2} = \sum_{n=0}^0 C_0 X^0 e^{-\alpha x^2/2} = C_0 e^{-\alpha x^2/2}$$

(45)

Multiplying (45) twice and integrating both sides result to the wave function for the harmonic oscillator in (33). The maximum value in $\psi_0(x) * \psi_0(x)$ when the slope is zero was obtain in (34). Considering Figure 2 below, it gives the Harmonic oscillator wave functions and probability densities.

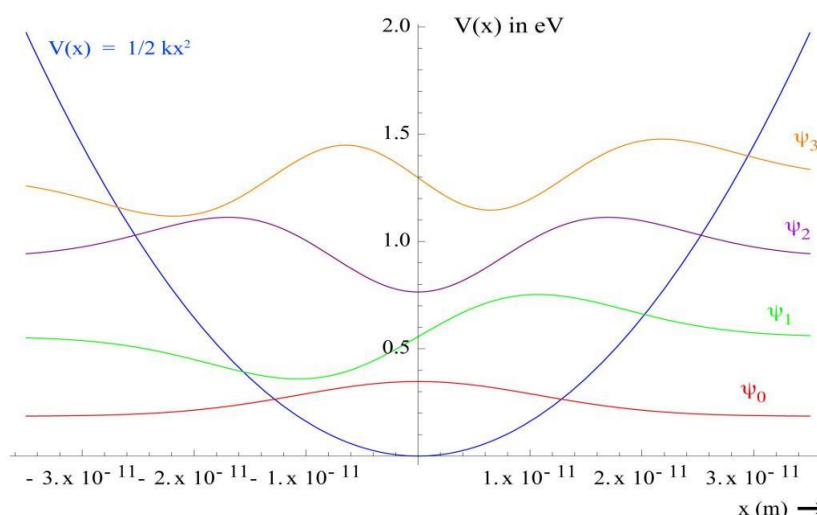
Wave functions

$$\psi_3(x) = \left(\frac{\alpha^3}{9\pi}\right)^{\frac{1}{4}} (2\alpha x^3 - 3x) e^{-\alpha x^2/2}$$

$$\psi_2(x) = \left(\frac{\alpha}{4\pi}\right)^{\frac{1}{4}} (2\alpha x^2 - 1) e^{-\alpha x^2/2}$$

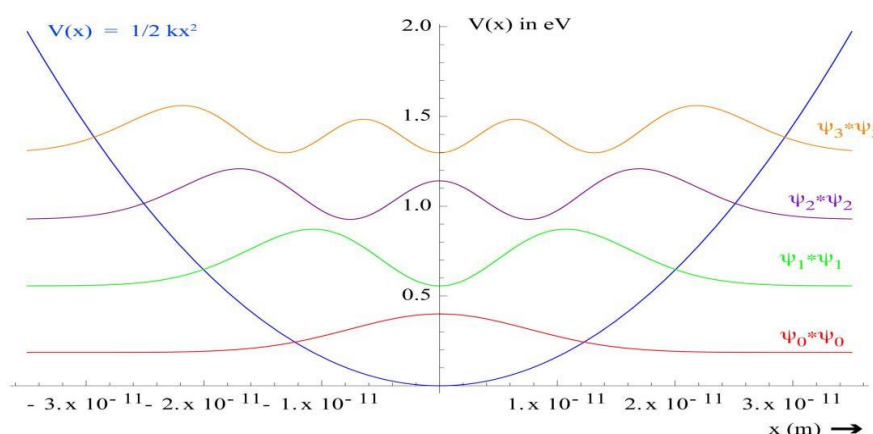
$$\psi_1(x) = \left(\frac{4\alpha^2}{\pi}\right)^{\frac{1}{4}} x e^{-\alpha x^2/2}$$

$$\psi_0(x) = \left(\frac{\alpha}{\pi}\right)^{\frac{1}{4}} e^{-\alpha x^2/2}$$



Plot of $V(x)$ and $\psi_n(x)$ for HCL

Harmonic Oscillator Probability Density



Plot of $V(x)$ and $\psi_n(x) * \psi_n(x)$ for HCL (using Matlab 2015a)

Figure 2: Harmonic oscillator wave functions and probability densities.

DISCUSSION

There are many different analytical approach to solving harmonic oscillator in one-dimension, the Nikiforov-Uvarov method is the most widely used because of its simplicity. However, very accurate results cannot be obtained by the method due to error arising from truncation, propagation, guessing of initial value to convert a boundary value problem to an initial value problem, the method was used by Lambert (2001) to model electron trapped in finite and infinite potential wells. The Schrodinger equation method is yet another method that gives an accurate result, the method has been applied to model diatomic molecules like H₂O, LiH and CO and

hydrogen chloride is the diatomic molecule in this case. Comparing the result in figure 2 with what is observed for a classical oscillator in Lambert (2001). A classical oscillator is moving fastest, or has the highest kinetic energy, when passing by the minimum in potential energy, i.e., the bottom of the well at $x=0$. For this reason, the classical oscillator spends the least time at the bottom of well and more time at the turn around points where its velocity drops to zero. The maximum probability of finding a classical oscillator is always along the edge of the well, not in the middle. However, that the probability of finding the quantum mechanical oscillator along the edge of the well improves with

increasing quantum number ν (see the progression of $\psi_\nu * \psi_\nu$ from $\nu=0$ to $\nu=3$ in figure 2). At large quantum numbers the classical and quantum mechanical oscillators correspond. This is referred to as the Correspondence Principle.

CONCLUSION

A lot of methods have been used to obtain solution for the harmonic oscillator. In this paper the Schrodinger equation is used to obtain the solution for the harmonic oscillator when compared to Lambert (2001) which uses same method together with boundary conditions and solved numerically. The Schrodinger equation gives clear understanding on the efficient and accuracy of results obtained when compared to other methods used to obtain solution for harmonic oscillator.

More researches should be done on the other methods of solution of harmonic oscillator such as numerical methods which involves computation with the use of software such as MATLAB etc.

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