Solving the one-dimensional Schrödinger Equation for the Harmonic Oscillator

V.H.G.Chávez
Faculty of Sciences, UANL
Computational Physics (Fall 2014)

The Harmonic Oscillator

The Harmonic Oscillator is a classical problem in mechanics and its generality is such that it enables us to model systems with attractive forces and any kind of vibrational phenomena, for example, the energy levels and transport properties of electrons in nanostructures, which are crucial in the development of the next generation of electronic devices. Besides, it allows us to have a fair understanding of the concept of quantization, its effects, and the wave function in bounded states.
This problem can be solved in an analytic manner, nevertheless, most of the practical problems of specific interest can only be solved using numerical approximations. In the following work we present an introduction to the general foundations of the time independent Schrödinger Equation for the resolution of the Harmonic Oscillator, then, a non-operator, mathematical approach is addressed and we conclude by the use of well known Numerov's algorithm for solving both the Differential Equation and the search of the energy eigenvalues.

The Schrödinger Equation

For a particle of a given mass 'm' under a symmetrical potential V(x), we find that the Schrödinger Equation in one dimension is:

$$\hat{H}\psi = E\psi \tag{1}$$

where $\hat{H}$ is the Hamiltonian for the Classic Harmonic Oscilator. We substitute and find:

$$\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) + V(x)\psi(x) = E\psi(x) \tag{2}$$

Then our main objective will be to find a solutions to the Second Order Differential Equation. It must be noted that most of the formal description of

the quantum theory is given by the use of linear operators but, this may not be the most convenient way of introducing the concepts. For this manner, the problem will be addressed in an approach that will try not to indulge in many of the abstraction of linear algebra. We will start with some definitions and theorems that are necessary for the proper development and understanding of the problem.

1. *Theorem*: In a one dimensional problem the energy levels of a bound state are *discrete* and non *degenerate* (we cannot, ever, find two different bounded states with the same energy value).

2. *Theorem* : The wave function $\psi(x)$ of a one-dimensional bound state has 'n' nodes ($\psi(x)$ *vanishes* n times).

The solution $\psi(x)$ is the wave function, which completely determines the state of a quantum object Also, we ought to consider some characteristics that $\psi(x)$ must satisfy:

1. $\psi(x) \in \mathbb{C}$

2. $\psi(x)$ is a differentiable hence continuous function

3. $\psi(x)$ is bounded, this implies that $\exists$ M such that $|\psi(x)|^2 \leq M$

The latter will be of great importance for the physical meaning of the solution, this is because that given any $\psi(x)$ there exist a probability associated with each value of the domain. The probability density is represented by the equation:

$$\mathbb{P} = \int |\psi(x)|^2 dx \tag{3}$$

From quantum theory we know that the energy values (eigenvalues) of the Energy operator are discrete, making the problem of not only of a differential equation nature given that we also need to figure out the values of the allowed energies. The resolution of the problem follows in the next section.

Solution to the Schrödinger Equation

The method here presented won't have exactly the formality which later on, with the historic development, came to solve using an operators method. This one though, is based on a series of manipulations done in the equation and in the subsequent results. The way it is solved is basically in three steps, making the DE adimensional → Asymptotic Analysis → Power Series. Let us begin:

Given the Time independent Schrödinger Equation (2) we find that most of the coefficients are physical quantities meaning that they carry along with them unities. It is convenient to remove them and deal only with numbers.

If we use the following change of variable:

$$x = \sqrt{\frac{\hbar}{mw}}u$$

and

$$E = \frac{\hbar w}{2}\epsilon$$

and we insert them in (1) we end up with the following adimensional Schrödinger Equation[1]:

$$\frac{d^2\psi(u)}{du^2} = (u^2 - \epsilon)\psi(u) \tag{4}$$

Now we can start doing some asymptotic analysis, consider the following:

$$\lim_{u\to\infty} u^2 - \epsilon \approx \lim_{u\to\infty} u^2$$

and we rewrite (for large values of u) the equation (4) as:

$$\frac{d^2\psi(u)}{du^2} = u^2\psi(u) \tag{5}$$

One can analyze equation (5) and notice that the only function that could behave in that manner would be the exponential function, furthermore, the only way we can obtain that solution is that if in the argument we obtain something like $\alpha\frac{u^2}{2}$. Let us then assume that the solution has the form:

$$\psi(u) = u^k e^{\alpha\frac{u^2}{2}} \tag{6}$$

where n is finite and n $\in \mathbb{N}$. By inserting (6) into (5) we can guarantee that the solution must behave in a similar manner[2], given that $\alpha = \pm 1$, now lets generalize and represent u^k as a $H(u)$ to find the general solutions to the DE:

$$\psi(u) = A_0 H(u) e^{\frac{+u^2}{2}} + A_1 H(u) e^{\frac{-u^2}{2}} \tag{7}$$

From the introduction, remember that our solution must be normalizable, thus our first part of the solution in (7) will quickly diverge, meaning that our particle would stop feeling the restoring force, while the second will converge in a manner that $|x| \to \infty$ then $\psi(u) \to 0$. We asume u^k is a well behaved function that does not grow faster that e^{u^2} otherwise we would end up again with a non-physical solution. By assuming that (6) is our solution, equation (4) becomes a differential equation in which our job now is to find the value of H(u):

$$H''(u) - 2uH'(u) + (2u - 1)H(u) = 0 \tag{8}$$

[1]The proof can be found in the Apendix
[2]The proof can be found in the Apendix

Suppose the solution can be expressed as a power series in the following manner:

$$H(u) = \sum_{n=0}^{\infty} a_n u^n \tag{9}$$

By deriving the latter and introducing them into (8) we can obtain a recursion formula[3] that will dictate the behavior of each of the coefficient of the infinite polynomials.

$$a_{n+2} = \frac{2n+1-\epsilon}{(n+1)(n+2)} a_n \tag{10}$$

It can easily be verified that all of our solutions will depend either on a_0 and a_1 (being a second order differential equations would be our initial conditions $H(0)$ and $H'(0)$) Again, let's assume we have an infinite number of terms (which comes from our premises) if we take n and make it very large a_{n+2} will behave like:

$$a_{n+2} \to \frac{2n}{n^2} a_n \tag{11}$$

It follows:

$$\frac{a_{n+2}}{a_n} \approx \frac{2}{n} \tag{12}$$

Now let us remember the Taylor expansion for the function:

$$e^{x^2} = \sum_{n=0}^{\infty} \frac{x^{2n}}{n!} = 1 + x^2 + \frac{x^4}{2!} + \frac{x^6}{3!} + \dots \tag{13}$$

Notice that all the exponents are even, then we can rewrite the sum as:

$$e^{x^2} = \sum_{n=2,4,6,\dots}^{\infty} \frac{1}{\frac{n}{2}!} x^n \tag{14}$$

Let us define $r = \frac{1}{\frac{n}{2}!}$ and propose the following:

$$\frac{r_{n+2}}{r_n} = \frac{\frac{1}{\frac{n+2}{2}!}}{\frac{1}{\frac{n}{2}!}} = \frac{\frac{n}{2}!}{\frac{n+2}{2}!} = \frac{\frac{n}{2}!}{(\frac{n}{2}+1)\frac{n}{2}!} = \frac{2}{n+2} \approx \frac{2}{n} = \frac{a_{n+2}}{a_n}$$

This means that our solution will behave as a e^{x^2}, which is exactly what we were trying to avoid since it would mean that we have a non-physical solution. Nevertheless, remember that our nth coefficient a_{n+2} has an unknown value ϵ corresponding to the energy. Since we also needed to determine the value of the energy we can manage to make the nth term vanish by making the numerator in (10) equal zero. We see that:

$$2n + 1 - \epsilon = 0 \Rightarrow \epsilon = 2n + 1$$

[3]Proof in the appendix

But remember how we defined Energy in (n). Using the result obtain before, we can find that:

$$E = \hbar w(n + \frac{1}{2}), \tag{15}$$

where n $\in \mathbb{N}$.

This means that Energy has discreet values! And the allowed energies are thus quantized. Later in the theory, the polynomials corresponding to the solution are defined as the *Hermite polynomials*. $H_n(u)$ is of degree n and thus has n zeroes. Then we have that the complete solution to the harmonic oscillator:

$$\psi_n(u) = H_n(u)e^{\frac{-u^2}{2}} \tag{16}$$

Numerical Solution to the Problem

The Numerov's algorithm (from its creator Russian Astronomer Boris Vasilyevich Numerov) is a very elegant yet particularly simple and efficient method (it works even better than the well known Runge-Kutta Method) for solving Second Order Differential equation in which the "first order" term is missing as follows:

$$\frac{d^2y}{dx^2} = k(x)^2y(x) + s(x) \tag{17}$$

The numerical solution here presented is based on the assumption that our equation can be discretized. Suppose that our solution exist in a certain domain (sufficiently large for our solution to converge) surrounding the origin for this, we select N divisions of a given length h. Then by multiplying $N * h$ we are able to get the values for the x_{max} in which our solution will exist, accordingly every value of our function will be given by $\psi(h_i)$, in the same fashion, will obtain the values for $k(h_n)$ and $s(h_n)$ (which in this case is zero).

It follows from the representation of the Taylor Expansion that the recursive equation for the nth term is found as (the proof can be found in the literature referenced below):

$$y(x)_{n+1} = \frac{2y_n[1 - \frac{5}{12}k_nh^2] - y_{n-1}[1 + \frac{1}{12}h^2k_{n-1}]}{[1 + \frac{1}{12}h^2k_{n+1}]} \tag{18}$$

Where:

$$k_n = \frac{2m}{\hbar^2}[E - V(h_n)]$$

Using it to Solve the Schrödinger Equation

Using the previously obtain value, we could easily find the solution. But we must consider before applying it that in order to use the algorithm first, we ought to have the first and second value of the function. This is analogous

to having our two initial conditions in any other differential equation problem. Consider though the boundary conditions that tells us that both:

$$\psi(h_0) = \psi(h_N) = 0$$

.

Then iteratively we can integrate to find the value of the function in each of the h_n, this will be for us particularly helpful since we know that our function must start with a value that $\to 0$ and a value that converges $\to 0$. With this in mind we can then set our initial values as this: $\psi(h_0) = 0$ and $\psi(h_1) = \varepsilon$ where ε is a number sufficiently small suited for the length of the integration area.

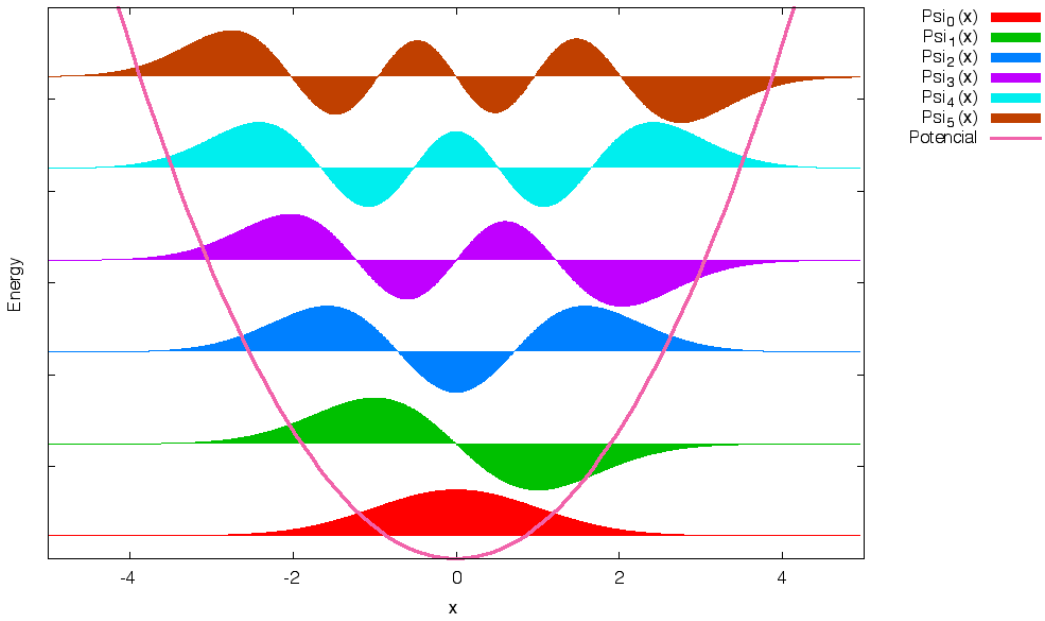
Parallel to obtaining the solution to the DE, it must also be noticed that not every value of the Energy will give a proper solution, making some results (actually most of them) diverge into values that are unwanted. This implies that we also need to find a way to obtain all the values of Energy that satisfy our conditions. For the latter we set a number of eigenvalues to find, latter, we set an initial value of it and we let the computer integrate solutions for the DE increasing each time the value of energy by a small value. Then, each of the ending values of each solution are compared to a very small quantity that verifies the solution. If the nth value is smaller than it, *it becomes a solution*. Eventually, when the solutions are found, the program must be able to normalize the results given, in our case we arbitrarily set to normalize to one.

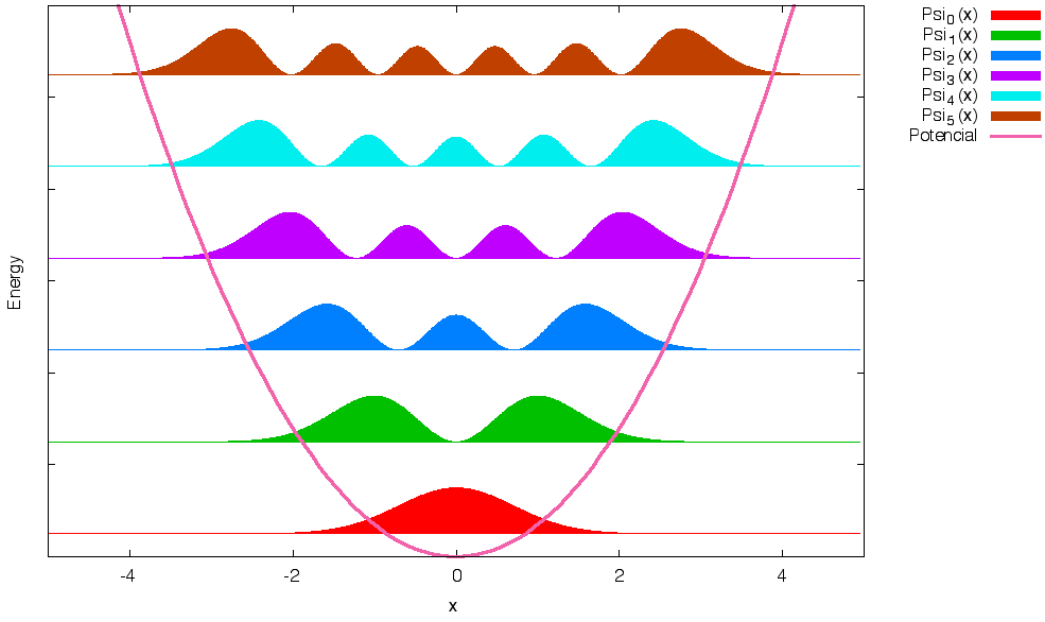
We continue with a code [Numeq.for] using the previous statements using the language Fortran. It is a code that provides a suited way of finding several of the first levels of energy. It must be noticed that the code is a convenient approximation and it definitely needs to be improved.

After a few test it is convenient that someone tries the following in order to get results that are coherent.

1. Values of x_{max} work best when is $\in$ [5:10]
2. N must be in the range of hundreds (one may increase the value above that, but the convergence should already have been achieved). Hence you then select a value of h to agree with (1).

Anyhow, the code prints out in the console all the values of the required number of eigenvalues for Energy. It also prints out two files, one with the data of (x,$\psi(x)$) of the number of solutions as well as another with the data (x,$\psi(x)^2$)as indexes for easy plotting using programs such as *gnuplot*. In this document we present the result of the previous program plotted using gnuplot with its respective discussion.


Psi0 (x)
Psi1 (x)
Psi2 (x)
Psi3 (x)
Psi4 (x)
Psi5 (x)
Potencial
Energy
-4
-2
0
2
4
x


Psi0 (x)
Psi1 (x)
Psi2 (x)
Psi3 (x)
Psi4 (x)
Psi5 (x)
Potencial
Energy
-4
-2
0
2
4
x

1. In the first plot we find that the solutions to the Schrödinger Equation. Each of the successive curves represents a state, notice how each of the states is congruent with the Node theorem that stated that it equals the number of nodes (or zeros) of each of the states. This is how we can graphically represent that the Energy cannot have a continuous spectrum.

2. In the second one we can find the physical real value of $\psi(x)$ all of those functions must be normalized to 1, thus the probability of finding the particle in the integrated region depends on where it is, and it must be inside the region of the Potential.

Apendix

(a) - Adimensional Schrödinger Equation

From the time-independent Schrödinger Equation

$$\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) + V(x)\psi(x) = E\psi(x)$$

We need to determine a series of variables that are a-dimensional in order to mathematically simplify the resolution of the equation. For that we assume the new variables will behave like:

$$x = u_0 u$$
$$E = \frac{1}{2}\epsilon_0 \epsilon$$

Where the *subterms* u_0 and ϵ_0 represent the coefficients that will vanish the current dimensions.
Re-writing the Schrödinger Equation and letting the potential be represented by $V(x) = \frac{1}{2}mw^2x^2$

$$\frac{d^2}{dx^2}\psi(x) = \frac{2m}{\hbar^2}(E - \frac{1}{2}mw^2x^2)\psi(x)$$

We insert the new defined variables.

$$\frac{d}{du}((\frac{d}{du}\psi(x))\frac{1}{u_0})\frac{1}{u_0} = \frac{2m}{-\hbar^2}(\frac{1}{2}\epsilon_0\epsilon - \frac{1}{2}mw^2u_0^2u^2)\psi(x)$$

And reduce to get:

$$\frac{d^2}{du^2}\psi(x)(\frac{1}{u_0^2}) = \frac{m}{\hbar^2}(\epsilon_0\epsilon - mw^2u_0^2u^2)\psi(x)$$

Since we only want to preserve the variables we suppose that $\epsilon_0 = mw^2u_0^2$:

$$\frac{d^2}{du^2}\psi(x) = \frac{mu_0^2}{\hbar^2}(mw^2u_0^2)(u^2 - \epsilon)\psi(x)$$

We then make:

$$m^2 w^2 u_0^4 = \hbar^2$$

And since:

$$[\hbar] = \frac{[x^2][m]}{[t]}$$

We can define:

$$u_0^4 = \frac{\hbar^2}{m^2 w^2}$$

Let us remember that we previously defined ϵ_o, then it follows:

$$\epsilon_0 = m w^2 (\frac{\hbar}{mw}) \Rightarrow \epsilon_0 = \hbar w$$

$\therefore$ The dimensionless Schrödinger Equation is:

$$\frac{d^2}{du^2}\psi(x) = (u^2 - \epsilon)\psi(x)$$

$\mathbb{Q}.\mathbb{E}.\mathbb{D}.$

Sketching the Solution

Let us plug $\psi(u) = u^k e^{\alpha \frac{u^2}{2}}$ into $\frac{d^2}{du^2}\psi(x) = u^2\psi(u)$. Then:

$$\psi(u) = u^k e^{\alpha \frac{u^2}{2}}$$

$$\psi'(u) = u^k(\alpha u)e^{\frac{\alpha u^2}{2}} + k u^{k-1} e^{\frac{\alpha u^2}{2}}$$

$$\psi''(u) = u^k(\alpha^2 u^2)e^{\frac{\alpha u^2}{2}} + 2(k u^{k-1})(\alpha u e^{\frac{\alpha u^2}{2}}) + (k)(k-1)u^{k-2}$$

Nevertheless, remember that we were doing an asymptotic analysis, that means that if we take $u \to \infty$ the terms with the largest degree will dictate the behavior of the function itself. Then:

$$\psi''(u) = (u^2\alpha^2)(u^k e^{\frac{\alpha u^2}{2}}) = u^2\alpha^2\psi(u)$$

And if we consider that $\alpha = \pm 1$ we have exactly what we were looking for in the first place. Then we prove that our selection of $\psi(u)$ was accurate.

Solving Differentail Equation for the Hermit Polinomyals

By inserting the suggested ψ into the adimensional differential equation we find (Here we modify the variable $u(x)$ as H):

$$\frac{d^2H}{du^2} - 2u\frac{dH}{du} + (\epsilon - 1)H = 0$$

Suppose that exist a solution in the form of a power series:

$$H(u) = \sum_{n=0}^{\infty} a_n u^n$$

$$H'(u) = \sum_{n=0}^{\infty} n(a_n)(u^{n-1}) = \sum_{n=1}^{\infty} n(a_n)(u^{n-1})$$

$$H''(u) = \sum_{n=0}^{\infty} (n)(n-1)(a_n)(u^{n-2}) = \sum_{n=2}^{\infty} (n)(n-1)(a_n)(u^{n-2})$$

It follows that:

$$\sum_{n=0}^{\infty} (n+2)(n+1)(a_{n+2})(u^n) - 2\sum_{n=0}^{\infty} n(a_n)(u^n) + (\epsilon - 1)\sum_{n=0}^{\infty} a_n u^n$$

$$\sum_{n=0}^{\infty} [(n+2)(n+1)a_{n+2} - (2n+1-\epsilon)a_n]u^n = 0$$

Since $n \in \mathbb{N} \Rightarrow u^n \neq 0$ And the coefficient must consistently vanish for any n.

$$\Rightarrow (n+2)(n+1)a_{n+2} - [2n+1\epsilon]a_n = 0$$

$$\therefore a_{n+2} = \frac{2n+1-\epsilon}{(n+2)(n+1)} a_n$$

$\mathbb{Q}.\mathbb{E}.\mathbb{D}.$

References

[1]Dirac, P. A. M. (1930). The principles of quantum mechanics.

[2]Shankar, Ramamurti, Ravi Shankar, and Ramamurti Shankar. Principles of quantum mechanics. Vol. 233. New York: Plenum Press, 1994.

[3]Allan Adams, Quantum Physics 804, Spring 2013. (Massachusetts Institute of Technology: MIT OpenCouseWare), http://ocw.mit.edu. License: Creative Commons BY-NC-SA

[4]Pang, Tao. An introduction to computational physics. Cambridge University Press, 2006.

[5]Koonin, Steven E., and Dawn C. Meredith. Computational physics. Addison-Wesley, 1990.

[6]Ginnasti, Paolo. Numerical Methods in Quantum Mechanics. Free Distribution, 2013.

[7]Pillai, M., Goglio, J., Walker, T. G. (2012). Matrix Numerov method for solving Schrdinger's equation. American Journal of Physics, 80(11), 1017-1019. Chicago.

[8]Anders W. Sandvik, Numerical Solutions of the Schrödinger Equation, Computational Physics PY 502, Fall 2013. Department of Physics, Boston University.

[9]Jorgensen, L., Cardozo, D. L., Thibierge, E. Numerical Resolution Of The Schrödinger Equation.