(a) Harmonic Oscillator: A Third Way

Introduction

This paper brings to attention the use of matrix to tackle time independent problems. There are other ways to solve time independent problems such as the differential equation method and the algebra method. The former involves a lot of algebra and makes use of power series as well. The latter method makes use of partial differential equations and Fourier transform. A typical problem is the infinite square well. A typical set up is made of three components, the free particle, the infinite square well and the Harmonic oscillator potential. The goal is to determine the relationship between the stiffness of the harmonic oscillator and the Eigen states. Stiffness is represented by a dimensionless parameter $(\frac{\hbar\omega}{E_1})$.

I will also show how to convert the Hamiltonian matrix into a simpler matrix that can be easily diagonolized and compare that result with what we have in the book. In the case of the free particle we shall consider a particle confined to the space enclosed by the walls of the well. The Quantum harmonic oscillator is analogous to the classical harmonic oscillator; furthermore it is one of the few systems for which a simple exact solution is known. A harmonic oscillator is a particle that is subject to a restoring force that is proportional to the displacement of the particle. In classical physics this is given by

$F = ma = m\frac{d^2x}{dt^2} = -kx$……………………………………………………………………… (1)

(b)The Infinite Square Well

The infinite square well potential is given by

V(x) = 0 if 0 <x<a

∞ Otherwise

A Particle in this potential is completely free except at the two ends (x=0 and x=a) where an infinite force prevents it from escaping.

In the region from zero to a the wave function must be a solution of

$\frac{-\hbar^2}{2m} + \frac{d^2\psi}{dx^2} = E\psi(x)$ where v(x) =0

The solution to this differential equation is the free particle solution which is

$\psi(x) = Ae^{ikx} + Be^{-ikx} = 2mE$ $k = \sqrt{\frac{2m\varepsilon}{h}}$

But now we have to apply whatever boundary conditions we have. We know that continuity of the wave function insists that ψ(0) = ψ(a) = 0, so,

$\psi(0) = A + B$ and $A = -B$, therefore

$\psi(x) = Ae^{ikx} + Be^{-ikx} = A\sin(kx)$

ψ (a)=A sin (ka)-0= where Ka=nπ n= 0, 1, 2…….positive integersψ (x) =$\left\{A_n \sin\left(\frac{n\pi x}{a}\right) \text{if } 0 < x < a\right\}$

$\{0\}$ otherwise

When this function is diagonalized to solve for the constant A. we find that $A = \sqrt{\frac{2}{a}}$, thus $\psi(x)$ becomes;

$\psi(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right)$ n=1, 2, 3……

These are the normalized stationary states. The new general state solution is given by

$\psi(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right) e^{\frac{iEt}{\hbar}}$ Solving for the Energy, E in the above equation we get

$E_n = n^2 h^2 \pi^2 / 2ma^2$ .This represent the Eigen values where the quantum number n takes positive integers , n= 1, 2, 3……………..

This paper will briefly mention the steps followed to obtain the Hamiltonian matrix, and then show a detailed solution to this matrix. The Hamiltonian is given by, $H_m = \hbar^2/2m\, \partial^2 x \;\; /\partial x^2$ + v(x)

The next step is to find the Hamiltonian matrix, diagonalize this matrix and find the Eigen values, which are the energy values. I shall briefly highlight the steps involved in coming up with the Hamiltonian matrix. Starting with the Schrödinger equation (H+V)|ψ>=E| ψ> then apply general expansion of a wave function in terms of a complete set of basis states, | ψ >=$\sum_{m=1}^{\infty} c_m$ |ψ_m > we get, $\sum_{m=1}^{\infty} c_m (H+V)\,|\psi_m$ =E $\sum_{m=1}^{\infty} c_m\, |\psi_m$ >, if we take the inner product of this equation we get the matrix equation $\sum_{m=1}^{\infty} c_m\, H_{nm}$, Where H_{nm} =<Ψn| (Ho +V) |Ψm>=δ_{mn} $E_n + \frac{2}{a} \int_0^a dx\, \sin(\frac{n\pi x}{a})$V(x) $\sin(\frac{n\pi x}{a})$. This is the Hamiltonian matrix, where δ_{mn} is the Kronecker delta and v(x) = $\frac{1}{2}$m$\omega^2 x^2$. For easy calculation we shall divide v(x) by E_1 and insert it into the above integral before solving this integral.

$\frac{v(x)}{E_1} = \frac{\pi^2}{4}(\frac{\hbar\omega}{E_1})^2 \; (\frac{x}{a} - \frac{1}{2}\;)$ Therefore we obtain the new equation

$H_{nm} = \delta_{mn} \;\; E_n + \;\frac{2}{a} \int_0^a dx\, \sin(\frac{n\pi x}{a}) \frac{\pi^2}{4} \;(\frac{\hbar\omega}{E_1})^2 \;(\frac{x}{a} - \frac{1}{2} \;\;) \sin(\frac{m\pi x}{a})$ ……………………….. (1). we need to sole this equation in order to obtain the matrix h_{nm} whixh when it is diagonalized it gives the Eigen values. Where $h_{nm} = \frac{H_{nm}}{E_1} = \delta_{mn} \;\; [n^2 + \frac{\pi^2}{48}(\frac{\hbar\omega}{E_1})^2 \left(1 - \frac{6}{(\pi n)^2}\right] + (1 - \delta_{mn}\;\;)\,(\frac{\hbar\omega}{E_1})^2 g_{mn}$

Where $\delta_{mn} \;\; = \left(\frac{(-1)^{n+m}+1}{4}\;\;\right)\left(\frac{1}{(n-m)^2} - \frac{1}{(n+m)^2}\right)$

(c) Solving the Hamiltonian Matrix

First let us introduce a variable in order to have eqn (1) in like terms, let y = $\frac{x}{a}$, then $dy = \frac{dx}{a}$, so (1) becomes

$H_{nm} = \delta_{mn} \;\; E_n + \;\frac{2}{a} \;\; a \int_0^1 dx \;\; (\sin n\pi y) \frac{\pi^2}{4} \;\; (\frac{\hbar\omega}{E_1})^2 \;\; (\frac{x}{a} - \frac{1}{2} \;\;\;) \sin(m\pi y)$ (y- $\frac{1}{2}$)^2………………. (2)

Let $v_1 = \delta_{mn} \;\; E_n$ and $v_2 = \frac{\pi^2}{4} \;\; (\frac{\hbar\omega}{E_1})^2$, then the above eqn becomes

$H_{nm} = v_1 + 2v_2 \;\;\;\; \int_0^1 dx\; \sin(n\pi y)\; \sin(m\pi y)$ (y- $\frac{1}{2}$)^2. Since we have x and y in the above eqn (2) we need to apply the same trick as above in order to have everything in same terms. So, let z= y- $\frac{1}{2}$, then $dz = dy$, now we have

$H_{nm} = v_1 + 2v_2 \;\;\;\; \int_{-\frac{1}{2}}^{\frac{1}{2}} \sin[n\pi(z + \;\; \frac{1}{2})] \sin[m\pi\,(z + \;\; \frac{1}{2})]\; z^2 dz$……………………………… (3), then by trig. Identity we can express,$\sin[n\pi(z + \;\;\frac{1}{2})] = \;\sin(n\pi z)\;\cos(\frac{n\pi}{2}) + \sin(\frac{n\pi}{2})\cos(\frac{n\pi}{2})$, therefore eqn (3) becomes, $H_{nm} = v_1$

$+2v_2 \;\; \int_{-\frac{1}{2}}^{\frac{1}{2}} [\sin(n\pi z)\; \cos(\frac{n\pi}{2}) + \sin(\frac{n\pi}{2})\cos(\frac{n\pi}{2})]\; z^2 [\sin(m\pi z)\; \cos(\frac{m\pi}{2}) + \sin(\frac{m\pi}{2})\cos(\frac{m\pi}{2})] dz$…………. ……………………………………………………………………………………………….. (4)

The next step is to come up with tables of $\cos(\frac{n\pi}{2})$ and $\sin(\frac{n\pi}{2})$ to simplify the above integral.

$\sin(\frac{n\pi}{2})$	1	0	-1	0

n	0	1	2	3

$\cos(\frac{n\pi}{2})$	0	1	2	3
n	0	1	0	-1

Using the above tables, eqn (4) simplifies to;

H_{nm} $=v_1$ $+2$

$$v_2 \int_{\frac{-1}{2}}^{\frac{1}{2}} [\cos(n\pi z)\ \sin(\frac{n\pi}{2}) + \cos(\frac{n\pi}{2})\ \sin(n\pi z)]\, z^2 [\sin(m\pi z)\ \cos(\frac{m\pi}{2}) + \sin(\frac{m\pi}{2}) \cos(m\pi z)] dz \text{...........}$$

.... (5)

We need to consider eqn (5) for the following cases

a. m and n are odd
b. m and n are even
c. m is odd, n is even
d. n is odd, m is even

For the cases c and d the integral evaluates to zero, while for both odd and both even cases the integral evaluates to the same answer. Therefore we shall consider only the latter case. For the case when m and n are both even eqn (5) reduces to;

$$H_{nm} = v_1 + 2\, v_2 \int_{\frac{-1}{2}}^{\frac{1}{2}} [\sin(n\pi z)\ \cos(\frac{n\pi}{2})]\, z^2 [\sin(m\pi z)\ \cos(\frac{m\pi}{2})]\, dz \text{...} \quad (6)$$

Since $\cos(\frac{n\pi}{2})$ and $\cos(\frac{m\pi}{2})$ does not depend on z, we pull it out of the integral. So we have;

$$H_{nm} = v_1 + 2\, v_2\, [\cos(\frac{n\pi}{2}) \cos(\frac{m\pi}{2}) \int_{\frac{-1}{2}}^{\frac{1}{2}} [\sin(n\pi z)]\, z^2 [\sin(m\pi z)]\, dz \text{..} \quad (7)$$

We can express the constant $\cos(\frac{n\pi}{2}) \cos(\frac{m\pi}{2})$ in a much simpler series form by using the table below and figuring out the pattern.

n	$\cos(\frac{n\pi}{2})$	m	$\cos(\frac{m\pi}{2})$
2	-1	2	-1
4	1	4	1
6	-1	6	-1
8	1	8	1
10	-1	10	-1

It follows that $\cos(\frac{n\pi}{2}) \cos(\frac{m\pi}{2})$= m $(-1^{\frac{m+n}{2}})$, the next part is to solve $\int_{\frac{-1}{2}}^{\frac{1}{2}} [\sin(n\pi z)]\, z^2 [\sin(m\pi z)]\, dz$, by using trig identity this equation becomes;

$$\int_{\frac{-1}{2}}^{\frac{1}{2}} (\cos[\pi z\,(n-m)] - \cos[\pi z\,(n+m)])\, z^2\ dz \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots . (8)$$

, let $p_1 = n - m$, $p_2 = n + m$ then (8) becomes

$$\frac{1}{2}\int_{\frac{-1}{2}}^{\frac{1}{2}} \cos[\pi z\, p_1]\ z^2\ dz - \frac{1}{2}\int_{\frac{-1}{2}}^{\frac{1}{2}} \cos[\pi z p_2]\, z^2\ dz \text{..} (9)$$

At this point we only need to solve one of the above integrals and the result will apply to both intergrals since they are similar except for the even integers . We shall use integration by parts twice.

$\frac{1}{2}\int_{\frac{-1}{2}}^{\frac{1}{2}} \cos[\pi z\, p_1]\ z^2\ dz$, let $u=z^2$, then $du = 2zdz$

Let $dv=\cos[\pi z\, p_1]dz$, then $\sin(p_1 \pi z)\frac{1}{p_1\pi}$ so now we have

$\frac{z^2}{p_1\pi}\sin(p_1\pi z) - \frac{2}{p_1\pi}\int_{\frac{-1}{2}}^{\frac{1}{2}} \sin[\pi z\, p_1]\ z\ dz$ .... (10), from here we need to use integration by parts the second time.

Let u= z then du=dz let $dv=\sin[\pi z\, p_1]dz$, $v = -\frac{\cos[\pi z p_1]}{p_1\pi}$, then we have

$-\frac{z}{p_1\pi}\ \cos\ [p_1\pi z]\ + \frac{\sin(p_1\pi z)}{(p_1\pi)^2}$ (10) becomes, $\frac{z^2}{p_1\pi}\sin(p_1\pi z) - \frac{2}{p_1\pi}[-\frac{z}{p_1\pi}\ \cos\ [p_1\pi z]\ + \frac{\sin(p_1\pi z)}{(p_1\pi)^2}]$

Evaluating (10) from $\frac{-1}{2}$ to $\frac{1}{2}$, we get;

$\left[\frac{\frac{1}{4}}{p_1\pi}\sin\left(\pi\ \frac{p_1}{2}\right) + \frac{1}{(p_1\pi)^2}\ \cos(\pi\ \frac{p_1}{2}) - \frac{2}{(p_1\pi)3}\ \sin(\pi\ \frac{p_1}{2})\right] - \left[\frac{\frac{1}{4}}{p_1\pi}\sin\left(\pi\ \frac{-p_1}{2}\right) + \frac{-1}{(p_1\pi)^2}\ \cos(\pi\ -\frac{p_1}{2}) - \frac{2}{(p_1\pi)3}\ \sin(\pi\ -\frac{p_1}{2})\right]$. This integral simplyfies to

$-[\frac{1}{(p_1\pi)^2}\cos(\pi\ \frac{p_1}{2}) + \frac{1}{(p_1\pi)^2}\cos(\pi\ \frac{-p_1}{2})$ ... ... (11)

Since Cosine is an even function and also $\frac{p_1}{2}$ is an even function. Let us simplify (11) using the table below

p_1	$\cos(\pi\ \frac{p_1}{2})$	$\cos(\pi\ \frac{-p_1}{2})$
2	-1	-1
4	1	1
6	-1	-1

From this table $\cos(\ \pi\ \frac{p_1}{2})$ takes the form $(-1^{\frac{p_1}{2}})$ and so (11) reduces to $(-1)^{\frac{p_1}{2}} + (-1)^{\frac{p_1}{2}}$ .... (12)

Solving (12) we get, $2\ \frac{-1^{\frac{n-m}{2}}}{\pi^2(n-m)^2}$ .... (13) Since $p_1 = n-m$. (13) is the result of the first integral of eqn (9), similarly the result of the second integral in eqn (9) would be, $2\ \frac{-1^{\frac{n+m}{2}}}{\pi^2(n-m)^2}$ .... (14)

Combining the two results according to eqn (9) we get,

$\frac{1}{2}[2\ \frac{-1^{\frac{n-m}{2}}}{\pi^2(n-m)^2}] - \frac{1}{2}\ [2\ \frac{-1^{\frac{n+m}{2}}}{\pi^2(n-m)^2}], = \frac{1}{\pi^2}[\ \frac{-1^{\frac{n-m}{2}}}{(n-m)^2} - \frac{-1^{\frac{n+m}{2}}}{(n-m)^2}]$.. (15)

Eqn (7), $H_{nm} = v_1 + 2\, v_2\, [\cos(\frac{n\pi}{2})\cos(\frac{m\pi}{2})\ \int_{\frac{-1}{2}}^{\frac{1}{2}} [\ \sin(n\pi z)\ ]\, z^2 [\ \sin(m\pi z)\ ]\, dz$ now becomes

$H_{nm} = v_1 + 2\, v_2\, [-1^{\frac{n+m}{2}}(\frac{-1^{\frac{n-m}{2}}}{\pi^2(n-m)^2} - \frac{-1^{\frac{n+m}{2}}}{\pi^2(n-m)^2}\ )]$ .... (16)

Since we already know that, $v_1 = \delta_{mn}\ \ E_n$ and $v_2 = \frac{\pi^2}{4}\ (\frac{\hbar\omega}{E_1})^2$, then (16) becomes

$H_{nm} = \delta_{mn}\ \ E_n + 2\,\frac{\pi^2}{a}\ [(\frac{\hbar\omega}{E_1})^2\ \frac{\pi^2}{4}\ ][-1^{\frac{n+m}{2}}][(\frac{-1^{\frac{n-m}{2}}}{\pi^2(n-m)^2} - \frac{-1^{\frac{n+m}{2}}}{\pi^2(n-m)^2}\ )]$...
(17)

For the special case where m=n, (17) becomes;

$H_{nm} = \delta_{mn} \; (n^2 + \frac{2}{a} \frac{\pi^2}{4} (\frac{\hbar\omega}{E_1})^2 \, [-1^{\frac{2n}{2}}][\frac{1}{24} - \frac{1}{4}(\frac{1}{(n\pi)^2})]\frac{24}{24}$ which gives;

$H_{nm} = \delta_{mn} \; (n^2 + \frac{\pi^2}{4} (\frac{\hbar\omega}{E_1})^2 \, \frac{1}{24} [-1^n] \, [1- \frac{6}{\pi n^2}] + (\frac{\hbar\omega}{E_1})^2 \, [1 - \delta_{mn} \;] g_{nm}$... (18)

Where

$g_{nm} = (\frac{-1^{n+m}}{4} \, (\frac{1}{(n-m)^2} - \frac{1}{(n+m)^2}))$

when equation (18) is diagonalized we get the Eigen values which represent the energies. These energies are plotted against the quantum numbers to produce the graph. I also plotted the graphs for different values of the unit less parameter to see the effect of the parameter on the solutions of both the harmonic oscillator and the infinite square well. At this point then expectation is that for low lying states of the unit less parameter the solution should be identical to that of the harmonic potential alone while for high energy states the solution should resemble those of the infinite square well. Using mathematica software to diagonlaize (18) and plot graphs different graphs.

Interpreting the Graphs

For larger values of $\frac{\hbar\omega}{E_1}$. when the harmonic oscillator is very stiff then the harmonic oscillator Eigen values well describes the low lying states. On the other hand if the harmonic potential is very stiff, i.e. low values of $\frac{\hbar\omega}{E_1}$ say $\frac{\hbar\omega}{E_1} = 1$, then instead of the Eigen states describing a harmonic oscillator states, there will be small perturbations of from infinite square well Eigen states. However it is important to note that this anomaly can be corrected by choosing a much wider infinite square well. I have attached some graphs.

Summary

The goal of this paper was to show how to solve a harmonic oscillator in quantum mechanics using a third way, which is matrix diagonalization. Which we have successfully shown, by use of the mathematica software. We have also realized that the unit less parameter $\frac{\hbar\omega}{E_1}$ represents the stiffness the harmonic oscillator potential. Large values of $\frac{\hbar\omega}{E_1}$ represents stiff harmonic oscillator while small values, say $\frac{\hbar\omega}{E_1} = 1$ represents less stiff harmonic oscillator potential. For less stiff harmonic oscillator potential none of the Eigen states describes the harmonic oscillator potential.

I have also successfully arrived at the same result as the paper by Marsiglio in coming up with a different form of the Hamiltonian matrix, which was easy to diagonalize. This was arrived at by use of various techniques discussed in the paper such as integration by parts.

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1. D. J. Griffiths, *Introduction to quantum mechanics*, 2nd ed. (Pearson/Prentice Hall, Upper Saddle River, NJ, 2005)

2. F. Marsiglio, “Harmonic Oscillator in Quantum Mechanics: A third Way, “American Journal of Physics Vol. 77, No. 3, March 2009.