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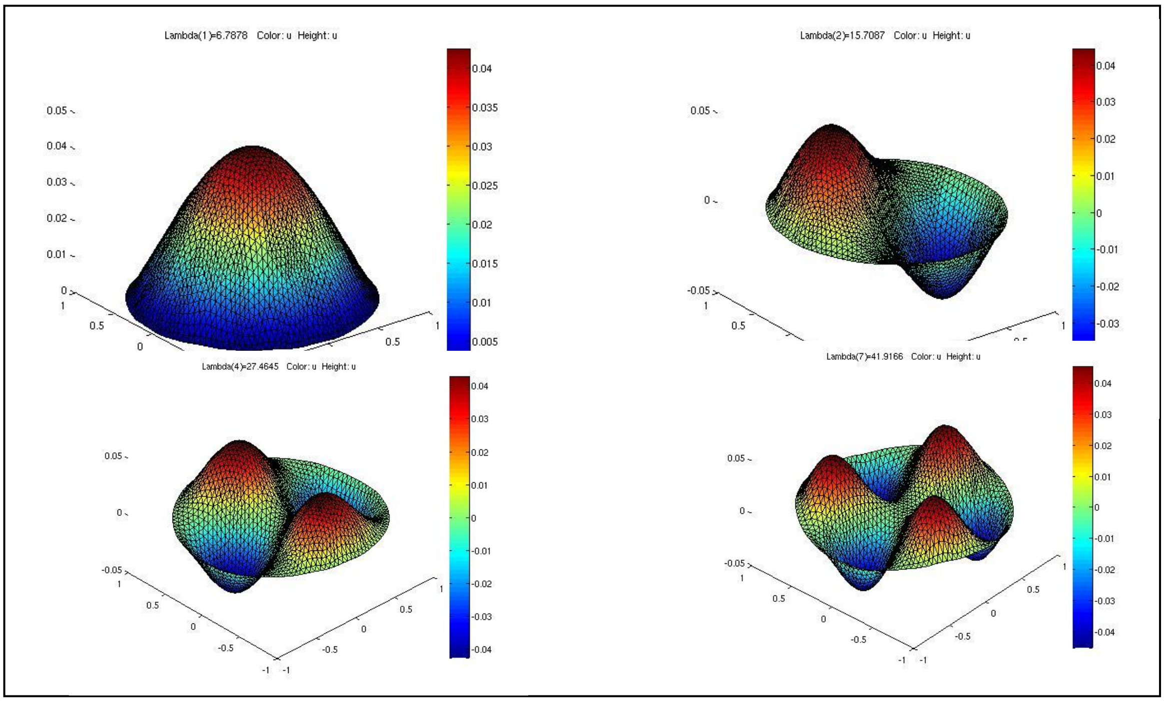

SOME ASPECTS ON THE SCHRÖDINGER EQUATION

AZHAR IQBAL

DEPARTMENT OF MATHEMATICAL SCIENCES

CHALMERS UNIVERSITY OF TECHNOLOGY

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AZHAR IQBAL

SUPERVISOR:

Prof. Nils Svanstedt

Department of Mathematical Sciences

Division of Mathematics

Chalmers University of Technology and University of Gothenburg

SE- 412 96 Gothenburg, Sweden

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Abstract

We consider various physical and mathematical aspects of the Schrödinger equation. We derive the linear time dependent Schrödinger equation with external potential. We also derive the Schrödinger eigenvalue problem and solve the eigenvalue problem numerically by a finite element method and a spectral method.

Acknowledgements

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Introduction

In this MSc thesis we are concerned with the Schrödinger equation. The Schrödinger equation is one of the fundamental equations in non-relativistic quantum mechanics. It describes the time evolution of a quantum state in e.g. atomistic or molecular configurations. It is an outstanding challenge to solve the Schrödinger equation. Analytical solutions are known only for very special "simple" atomistic configurations, like the Hydrogen atom. Also numerically the equation is a challenge, except for particle systems with not too many particles. In the present thesis we give a physical background of the Schrödinger equation and derive the linear Schrödinger equation from first principles. We then discuss various theoretical and technical aspects of the equations. In particular we derive the Schrödinger eigenvalue problem starting from a time dependent linear Schrödinger equation with time-independent potential. The analysis of the spectrum for the Schrödinger equations is one of the fundamental problems in quantum mechanics. The eigenvalues describe the energy state of e.g. an electron in a potential. The principal eigenvalue represents the ground state. We compute numerically the first eigenvalues for some one-dimensional and two-dimensional linear Schrödinger equations with small and large potentials by using two different numerical methods, a finite element method and a spectral method.

1. Quantum Mechanics Background

In the late 19th century classical theory of physics starts to face more and more contradictions and difficulties and it starts to become clear that phenomena on the atomic and subatomic scale do not fit into the framework of classical physics. The explanation of the phenomena on the atomic level has to be based upon entirely new principles. The foundation of these new principles will take place in stages as the result of many attempts. In the 1920s a coherent theory for microscopic phenomena is formed under the name of quantum mechanics.

In the universe one distinguishes two categories of objects, matter and radiation. Matter is made up of completely localized cells subject to Newton's laws of Mechanics, while on radiation obeys Maxwell's laws of electromagnetism. In contrast to matter, it is impossible to separate the radiation into corpuscles as it exhibits a wavelike behavior.

At the turn of the 19th century, the experimenters follow two closely related lines. One is to make a precise analysis of the microscopic structure of matter and second one is to determine the mutual interaction of material corpuscles and their interaction with the electromagnetic field. The first facts concerning the study of matters is performed by the study of the cathode rays in a discharge tube as the beams of electrically charged particles travel. In 1897 the electron was discovered experimentally by J. J. Thomson.

The existence of atoms and molecules appeared as in the study of Brownian motion, the irregular (random) motion suspended in a liquids or a gas and this study of motion of molecules can be quantitatively related to the statistical laws of motion of the molecules.

Difficulties appear when studying spectral distribution of magnitude radiation in thermodynamics equilibrium with matter. This occurs for instance in case of the black body that absorbs radiation. The spectral distribution of energy intensity is a measure of temperature. The expression deduced from classical theory contradicts the experimental results. In 1900 Max Planck removes this difficulty by giving the classical law of interaction between matter and radiation. Planck postulates that the energy exchanges between matter and radiation do not take place in continuous manner but by discrete and indivisible quantities or quanta of energy .He then shows that the quantum of energy must be proportional to the frequency ν of the radiation.

$$\varepsilon_{\upsilon} = h\upsilon, \tag{1.1}$$

where h is known as the Planck's constant.

Planck's hypothesis had to be confirmed by a complete collection of experimental facts which we agreement with the direct analysis of the elementary processes, and the direct revelation of the subsisten discontinuities in the revolution of physical systems on the microscopic scale, where classical theory pre a continuous evolution.

In 1905 A. Einstein explains the phenomena of photo electronic effect. He postulates that light radiation itself consists of a beam of corpuscles, the photons, of energy $h\upsilon$ and velocity c, ($c = 3 \times 10^{10}$ cm/sec). It is deducted experimentally that electric intensity is proportional to the intensity of radiation. While the velocity of the electron is independent the radiation intensity.

In 1924 Compton performed an experiment in which X-rays are scattered by free electrons. The wavelength of the Scattered radiation increases that of the incident radiation. The relation connecting the energy ε and the momentum p of a photon is

$$\varepsilon = pc. \tag{1.2}$$

Consider a plane monochromatic light wave

$$\exp\left[2\pi i\left(\frac{u.r}{\lambda} - \upsilon t\right)\right]. \tag{1.3}$$

According to Einstein's hypothesis this representing a stream of photons of energy $h\upsilon$ .the momentum is evidently directed along the velocity u and magnitude is

$$p = \frac{h\upsilon}{c} = \frac{h}{\lambda}. \tag{1.4}$$

The angular frequency $\omega = 2\pi\upsilon$ and the value of the wave vector is $k = \left(\frac{2\pi}{\lambda}\right)u$.

The relation between them is

$$\varepsilon = h\omega\,, p = \hbar k. \tag{1.5}$$

The corpuscles theory of the Compton effects describe that the total energy and momentum are sealed in the elastic collision among the electron and incident photon.

Figure no 1.1 shows the collision of photons with an electron at rest

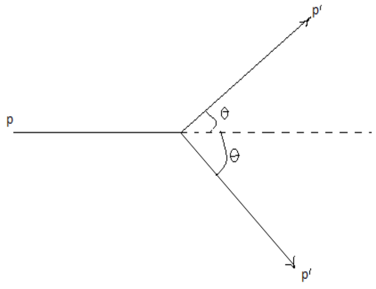

Figure no 1.1

The most important defect of the classical theory becomes transparent in the determination of the continuous transfer of momentum and energy of the radiation to all the electrons exposed to the radiation. Experiments indicate that this effect is discontinuous. There are two facts which are connected. One is that Compton scattering can be measured as light absorption and the other is that the photoelectric effect is a simple absorption.

If there will be some suggestion that the classical wave theory is macroscopically right , it is even so clear that on the microscopic scale only the absorption and scattering phenomena such as the photoelectric effect and Compton effect, respectively. One important thing is that single photons travel independently of each other and their jointly interaction is totally insignificant.

Light appears in two forms, one is of wave nature and the other is of corpuscle nature. These aspects appear in comparatively clear cut fashion depending upon the phenomena under consideration.

In 1923 according to N. Bohr, the atom does not behave as a classical system capable of exchanging energy in a continuous way. It can be present only in a definite number of stationary states or quantum states and each having a precise energy. One says that the energy of the atom is quantized. Energy can vary only by jumps from one position to another, each jumps corresponding to a transition.

From this postulate we can identify the method of absorption or emission of light through quanta. In the occurrence of light, an atom of energy E_i may go through a transition to a state of higher energy $E_j(> E_i)$ by absorbing a photon hυ provided that the total energy is preserved, that is

$$H\upsilon = E_j - E_i. \tag{1.6}$$

In the same way the atom can undergo a transition to a state of lower energy $E_k(< E_i)$ by emitting a photon hυ whose frequency satisfy the relation

$$H\upsilon = E_i - E_k. \tag{1.7}$$

Note that if the atom finds itself in its lowest energy position (ground state) it cannot radiate and remains stable.

In this way the existence of spectral lines characteristics of each atom is found and the principle of Rydberg -Ritz combination is satisfied, i.e. the spectral terms are equal up to a factor of h, to the energies of the quantum states of the atom. The energy levels are given by the formula

$$E_n = -\frac{hR}{n^2} \tag{1.8}$$

Physicists have analyzed the most important difficulties encountered by classical theory in the field of microscopic physics. These difficulties appear immediately if one makes a detailed study of the interaction between matter and radiation. The important effect is the appearance of discontinuity on this scale, combined with the existence of an indivisible quantum of action $\hbar$. On the atomic scale $\hbar$ ceases to be insignificant and characteristic quantum effects appear.

The simplest way to understand this wave corpuscle duality is to postulate a statistical bond connecting waves and corpuscles, where the intensity of the waves at a point gives the probability of finding the photon which is connected with it, at that point.

The failure of classical theory seems be the sole origin to the development of quantum theory.

2. The Schrödinger Equation

The Schrödinger equation was formulated in 1926 by the Austrian physicist Erwin Schrödinger. It describes how the quantum states of a physical system changes in time. It is also called a wave function or state vector. In pure mathematics, Schrödinger's equation and its variants are widely used in the field of partial differential equations. It has application in geometry, spectral and scattering theory and to integral systems.

The Schrödinger equation can be written in two different forms, the time dependent Schrödinger equation and the time independent Schrödinger equation.

The Time dependent Schrödinger equation is the most general form which gives a description of a system evolving with time and **the time independent Schrödinger equation** is sufficient when the systems in a stationary state.

For a general quantum system

$$i\hbar\frac{\partial}{\partial t}\psi = \hat{H}, \tag{2.1}$$

where

- ψ is the wave function
- $i\hbar\frac{\partial}{\partial t}$ is the energy operator
- i is the imaginary unit and $\hbar$ is the plank constant.
- $\hat{H}$ is the Hamiltonian operator.

  - **For a single particle in a potential**

    For a single particle the Schrödinger Equation with potential energy V reads

$$i\hbar\frac{\partial}{\partial t}\psi(x,t) = \hat{H}\psi = \left(-\frac{\hbar^2}{2m}\nabla^2 + U(x)\right)\psi(x,t) = -\frac{\hbar^2}{2m}\nabla^2\psi(x,t) + U(x)\psi(x,t), \tag{2.2}$$

where

- $-\frac{\hbar^2}{2\mathrm{m}}\nabla^2$ is the kinetic energy operator ,(m is the mass of the particle, ∇^2 is the Laplace operator).
- $U(\mathrm{x})$ is the time independent potential energy at the position *x*.
- $\psi(x,t)$ is the wave function for the particle at position *x* at time t.
- $\hat{H} = -\frac{\hbar^2}{2m}\nabla^2 + U(x)$ is the Hamiltonian operator for a single particle in a potential.

2.1 The Time Dependent Schrödinger Equation

When the particle of interest is confined to one spatial dimensional, the Schrödinger equation is used. For example the x-axis. We will start with the total energy equation to drive the one dimensional Schrödinger equation.

$$\frac{\mathrm{p}^2}{2\mathrm{m}} + \mathrm{U(x)} = \mathrm{E_{total}} \qquad (2.1.1)$$

where $\frac{\mathrm{p}^2}{2\mathrm{m}}$ is the kinetic energy and $\mathrm{U(x)}$ is the potential energy.

After substituting into the above equation we get the one-dimensional time independent Schrödinger wave equation

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x,t) + U(x)\psi(x,t) = -\frac{\hbar}{i}\frac{\partial}{\partial t}\psi(x,t). \qquad (2.1.2)$$

The L.H.S of (2.1.2) can be rewritten by using the Hamilton or total energy operator

$$H = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + U(x). \qquad (2.1.3)$$

By using the notation of Hamilton operator the Schrödinger equation reads

$$H\psi(x,t) = -\frac{\hbar}{i}\frac{\partial}{\partial t}\psi(x,t) \qquad (2.1.4)$$

As we know Schrödinger's equation is a partial differential equation for ψ in terms of two variables. By applying separable method

$$\mathrm{C} = \psi(x)\mathrm{f(t)} \qquad (2.1.5)$$

where $\mathrm{X(x)}$ is function of x only and $\mathrm{T(t)}$ is a function of t only. By inserting (2.1.5) into the Schrödinger equation we get

$$\frac{1}{\psi(\mathrm{x})}\mathrm{H}\psi(\mathrm{x}) = \frac{\mathrm{i}\hbar}{\mathrm{f(t)}}\frac{\mathrm{d}}{\mathrm{dt}}\mathrm{f(t)} \qquad (2.1.6)$$

- LHS is a function of x only.
- RHS is a function of t only.

Since changing t cannot effect LHS (changing x does not effect RHS), (2.1.6) can be separated into two separate ordinary differential equations.

Both sides must equal to the same separation constant so that

$$\frac{\mathrm{i}\hbar}{\mathrm{f(t)}}\frac{\mathrm{d}}{\mathrm{dt}}\mathrm{f(t)} = \mathrm{constant} \qquad (2.1.7)$$

where is constant =E (the meaning of E will become evident below.)

After integration of Eq. (2.1.7) we get the following result

$$\mathrm{F(t)} = \mathrm{e}^{-\mathrm{iEt}/\hbar}. \qquad (2.1.8)$$

By putting this result into (2.1.5), we obtain the equation for the time evolution

$$\psi(x,\mathrm{t}) = \psi(x)\mathrm{e}^{-\mathrm{iEt}/\hbar} \qquad (2.1.9)$$

To find the real quantity of the energy E, we compute the expectation value of the total energy by wave function obtained from the product method

$$\langle E_{total}\rangle = \int_{-\infty}^{\infty} \psi^*(x)\mathrm{f}^*(t)\left(-\frac{\hbar}{\mathrm{i}}\frac{\partial}{\partial \mathrm{t}}\right)\psi(x)\mathrm{f(t)d}x = \mathrm{e}^{\mathrm{iEt}/\hbar}\,\mathrm{e}^{\mathrm{iEt}/\hbar}\mathrm{E}\int_{-\infty}^{\infty}\psi^*(x)\,\psi(x)\mathrm{d}x = \mathrm{E} \qquad (2.1.10)$$

Since the wave function is normalized, i.e. $\langle\psi(x)|\psi(x)\,\rangle = 1,$ is the expectation of the total energy.

2.2 The time independent Schrödinger equation

This equation is obtained by inserting the wave function obtained from the product method, from (1.9) into the time independent Schrödinger equation

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) + U(x)\psi(x) = E\psi(x) \qquad (2.2.1)$$

which is the time independent Schrödinger equation. By using the Hamiltonian operator one obtains

$$H\psi(x) = E\psi(x). \qquad (2.2.2)$$

As H is an operator and E is a real number, the Schrödinger equation has the form of an eigenvalue equation. The eigenfunctions $\psi_n(x)$ and eigenvalues E_n are found by solving the Schrödinger equation.

E_n are discrete, i.e. only definite energy values are acceptable, all other energies are not allowed. The energy eigenvalues are also called eingenenergies or eigenstate energies.

2.3 One dimension Schrödinger equation for a Free Particle

The one-dimensional Schrödinger equation is

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + U(x,t)\psi = i\hbar\frac{\partial\psi}{\partial t}. \qquad (2.3.1)$$

This equation is a homogeneous and linear partial differential equation for the function $\psi = \psi(x,t)$, we know that $\hbar = \frac{\mathrm{h}}{2\pi}$, m is the mass of the particle and $U(x,t)$ is the potential.

We will use separable method to find the solution of $\psi(x,t)$ such that

$$\psi(x,t) = X(x)T(t). \qquad (2.3.2)$$

We substitute this into (2.3.2) and get

$$-\frac{\hbar^2}{2m}\frac{X''}{X} + U(x,t) = i\hbar\frac{T'}{T}\,. \qquad (2.3.3)$$

We assume now that the potential U is independent of time so that (2.3.3) becomes

$$-\frac{\hbar^2}{2m}\frac{X''}{X}+\ U(x)=i\hbar\frac{T'}{T}. \qquad (2.3.4)$$

From (2.3.4) we can see that the left hand side is a function of x only and right hand side is a function of t only so this equation will be equal to some constant, which we denote E. So the partial differential equation can be separated into two ordinary differential equations

$$T'=-i\frac{E}{\hbar}T(t), \qquad (2.3.5)$$

$$-\frac{\hbar^2}{2m}X''(x)+U(x)X(x)=\ EX(x) \qquad (2.3.6)$$

From (2.3.5) we get

$$T(t)=\ T_0e^{-i\frac{E}{\hbar}t}. \qquad (2.3.7)$$

We deduce from equation (2.3.7) that the angular frequency of oscillation is $\omega=\frac{E}{\hbar}$.

Now we will solve (2.3.6). The differential equation for X(x) has no solution until we identify the potential $U(x)$. But our concern only here is free particle one with no outside force. It means here that zero force implies a constant potential i.e. $U(x)=0$

After putting $U(x)=0$ (2.3.6) becomes

$$X''(x)+\ \frac{2mE}{\hbar^2}X(x)=0. \qquad (2.3.8)$$

This is a harmonic oscillator equation. From (2.3.8) we will get following two solutions

$$X^+(x)=\ X_0e^{i\sqrt{\frac{2mE}{\hbar^2}}x}, \qquad (2.3.9\text{ a})$$

$$X^-(x)=\ X_0e^{-i\sqrt{\frac{2mE}{\hbar^2}}x}. \qquad (2.3.9\text{ b})$$

In the wave vector k is the factor in the argument of the harmonic function. Hence $k=\sqrt{\frac{2mE}{\hbar^2}}$. Solving this equation for $E=\frac{\hbar^2k^2}{2m}$ and compare this with $\frac{E}{\hbar}$ we get

$$\omega(k)=\frac{\hbar k^2}{2m}. \qquad (2.3.10)$$

Note that as a function of k, this is different than

$$\omega(k)=ck. \qquad (2.3.11)$$

The scattering relation for harmonic solutions to the wave equation. Combining the equations for T and X we find two linearly independent solutions to the free particle Schrödinger equation

$$\psi_k^+(x,t)=\psi_0e^{ikx}e^{-i\omega t}=\psi_0e^{i(kx-\omega t)}=\psi_0e^{ik[x-(\frac{\omega}{k})t]}, \qquad (2.3.12\text{ a})$$

$$\psi_k^-(x,t)=\psi_0e^{-ikx}e^{-i\omega t}=\psi_0e^{-i(kx+\omega t)}=\psi_0e^{-ik[x+(\frac{\omega}{k})t]}. \qquad (2.3.12\text{ b})$$

2.4 The Three-Dimensional Schrödinger Equation

The three dimensional Schrödinger equation reads

$$i\hbar\frac{\partial}{\partial t}\psi = -\frac{\hbar^2}{2m}\left\{\frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2} + \frac{\partial^2\psi}{\partial z^2}\right\} + U(x)\psi. \tag{2.4.1}$$

This is the complete Schrödinger equation.

3. NON-RELATIVISTIC QUANTUM MECHANICS

3.1 Phase velocity and group velocity

If a group of two or more waves which have almost same frequencies are superimposed on each other the resultant wave will have different properties from those of the individual waves. The variation in the amplitude can be found in the resultant waves that represents the wave group or wave packet.

Consider a one dimensional wave

$$A(x,t) = A_0 e^{(kx-\omega(k)t)}, \tag{3.1.1}$$

where A_0 is the magnitude, k the wave number, $\omega(k)$ is the angular frequency and t is the time. Note that ω depends on the wave number k and we know that the wave length $\lambda = \frac{2\pi}{k}$. This phenomenon is called dispersion so we will starting from this $\omega(k)$

Phase velocity is define as

$$v_p = \frac{\omega}{k}. \tag{3.1.2}$$

We know that the phase velocity is the half of the classical velocity in free space and also note that the wave packets do not normally move with phase velocity. The velocity which help to move with is called the ¨group velocity¨ and is defined as

$$v_g = \frac{\partial\omega}{\partial k}. \tag{3.1.3}$$

Both are the same for linear dispersion with $\omega(k) = ak + b$. There are different kinds of dispersion relations but here we only consider the case of a free, non relativistic quantum mechanical particle of mass m , which is

$\omega(k) = ak + b$.

$$E(k) = \frac{\hbar^2 k^2}{2m} \ , \tag{3.1.4}$$

3.2 Catter-Anticatter model and the concept of particle and wave nature

Consider a particle fixed at O_0 in frame B as shown in figure (1) and the frame B travels in X direction at speed v with respect to lab frame A. Note that both X_o and X are parallel axes. For rotating motion of Catter and Anticatter the value of $\omega_0 = \frac{m_0}{\hbar} c^2$ .In frame the motion of rotating mass of either catter or anticatter along Y_0 axis

With $\theta_i = \omega_0 t_0$ can be described as

$$y_0 = A_0 \, sin(\omega_0 t_0) \, . \, \delta(x_0) \tag{3.2.1}$$

where A_0 denotes the amplitude which measured from the frame B. Note that $\delta(x_0) = \infty$ for $x_0 = 0$, The term $\delta(x_0)$ is only used to show that the disc is at $x_0 = 0$.

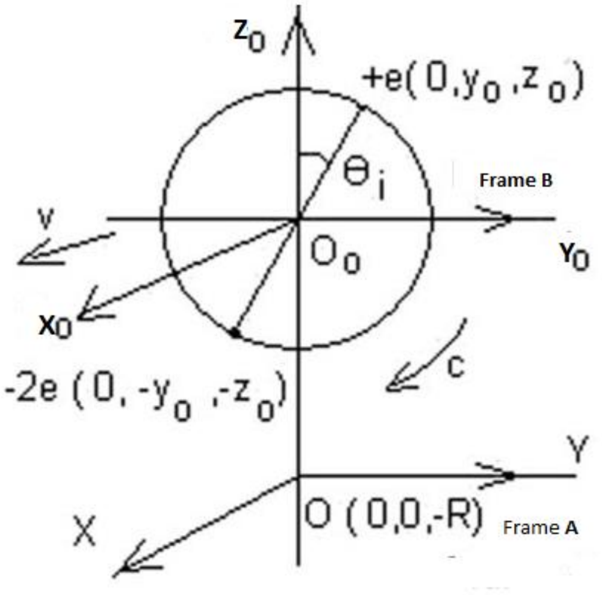

Figure 1

Now we consider x and t are measurements in frame A to see this oscillation in this frame

The relativistic transformation is

$$t_0 = \gamma(1 - xv/c^2). \tag{3.2.2}$$

and

$$x_0 = (x - vt). \tag{3.2.3}$$

Let A be the amplitude measured in frame A. The radius of Catter-Anticatter does not change as long as the plane of rotation of the disc is perpendicular to direction of motion i.e. X axis. So for rotating masses of Catter-Anticatter $A = A_0 = r_0$. By applying the property of delta function, at $x = vt$ we can write as

$$f(x, y)\delta(x - y) = f(a, y)\delta(x - a), \tag{3.2.4}$$

$$y = Asin(\gamma\omega_0(t - xv/c^2)).\delta(\gamma(x - vt)) = Asin\left(\omega_0 t\sqrt{1 - v^2/c^2}\right).\delta(\gamma(x - vt)). \tag{3.2.5}$$

The mass of the particle is localized at O_0 and $\omega = \omega_0/\gamma$ measured from frame A. For time dilation the masses of Catter-Anticatter are dependable by the particle nature. r0 does not change in the lab frame and the velocity of Catter-Anticatter disc is $Vin = r_0\omega_0/\gamma$. The value of c in particle frame is $c = r_0\omega_0$. By squaring the above equation can be written as

$$c^2 = V^2 in + v^2. \tag{3.2.6}$$

Multiply by $\gamma m_0(mc^2)$, where $m = \gamma m_0$. then the equation will be

$$E_M^2 = (mc^2)mc^2 = (\gamma m_0(c^2 - v^2) + mv^2)mc^2 = m_0^2 c^4 + p^2 c^2. \tag{3.2.7}$$

Particle energy $E_M = \pm mc^2$. This is the energy with the particle nature.

The Catter-Anticatter pair moreover has the rotating charges, which give rise to electric potential. A point charge e is localized at $x = x'$ described as e$\delta(x - x')$ and

$$\nabla'^2 \left(V\left(\vec{x} - \vec{x'}\right) \right) = \nabla'^2 \left(\frac{e}{4\pi\epsilon_0 \left|\vec{x} - \vec{x'}\right|} \right) = \frac{-e}{\epsilon_0} \delta\left(\vec{x} - \vec{x'}\right), \qquad (3.2.8)$$

where $V\left(\vec{x} - \vec{x'}\right)$ is a potential function which has a non-localized presence. Assume that we have a non-localized oscillating potential in frame B and we can write as $y_0 = A_0 sin\,(\omega_0 t_0)$. For measurements from A by a lab view, put t_0 and we get

$$y = Asin\gamma\left(\omega_0 t - \left(\frac{\omega_0 v}{c^2}\right) x\right), \qquad (3.2.9)$$

where A is a amplitude in frame A . Then for $\omega = \gamma\omega_0$ we will get a wave of the nature as

$$y = Asin(\omega t - kx). \qquad (3.2.10)$$

We know that $\lambda = 2\pi/k$ gives the de Broglie wave length $\lambda = h/p$ and phase velocity $v_p = \omega/k$ gives$v_p = c^2/v$.

Now we will discuss the case where there is a non-localized oscillation in particle frame B. Then we will get a wave in frame A. If we replace y with ψ then this wave satisfies the following general wave equation in frame A. which is

$$\frac{\partial^2\psi}{\partial x^2} = \frac{1}{v_p^2 \partial t^2}. \qquad (3.2.11)$$

The solution of the wave equation is

$$\psi = ae^{\pm\frac{i}{\hbar}(E_w t - px)} = ae^{\pm i(\omega t - kx)}. \qquad (3.2.12)$$

In order to use the relativity principles we require

(1) Object under study and
(2) The observer

For taking into account the electric field effect, the observer has to consider to be another charge. In the Hydrogen atom the proton has a point charge due to large mass is an observer which is considered as stationary in lab frame. Interaction energy is present in-between the proton and an electron which corresponds to their eigenstates. By using measuring instruments, the human observer in laboratory can determine the difference in energy between two eigenstates by observing the emission of photons.

Observation:

The particle energy with mass m in lab frame is $E_w = \gamma\hbar\omega_0$. The joining point for both types of nature is the energy. The energy equation is related to the particle nature and is called the classical mechanics equation and the energy related with the wave nature is called the quantum mechanical equation.

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3.3 Schrödinger equation for a particle in uniform potential

For a free particle as we discuss above $E_w = \gamma\hbar\omega_0$ and the kinetic energy is $= m_0v^2/2$. we know the value of $\omega_0 = m_0c^2/\hbar$ and for velocity $v << c$, the solution of the wave equation is

$$\psi = ae^{\pm\frac{i}{\hbar}(E_wt-px)} = ae^{-i(\gamma\omega_0t-kx)} \cong ae^{-i(\omega_0t(1+\frac{v^2}{2c^2})-kx)} = a^{-i\omega_0t}e^{-i(\frac{\omega_0tv^2}{2c^2})-kx)} = ae^{-i\omega_0t}e^{-i\left(\frac{E}{\hbar}t-\frac{p}{\hbar}x\right)} . \quad (3.3.1)$$

So we can write $\psi = a\psi_{t_0}\psi_s$ (3.3.2)

where $\psi_{t_0} = a^{-i\omega_0t}$ *and* $\psi_s = e^{-i\left(\frac{E}{\hbar}t-\frac{p}{\hbar}x\right)}$.

After differentiating (3.3.2) we will find $\partial^2\psi/\partial x^2$ and $\partial^2\psi/\partial t^2$ and then we will put this result in the equation which we derived in previous section. Cancel $a\psi_{t_0}$ and neglected the terms with $(v^2/c^2\ )$ *and* v^4/c^4 .

$$\frac{\partial^2\psi_s}{\partial x^2} = -\frac{m_0^2v^2}{\hbar^2}\psi_s = \frac{-2m_0}{\hbar^2}(E\psi_s). \quad (3.3.3)$$

After differentiating ψ_s we get

$$(E\psi_s) = -\frac{\hbar}{i}\frac{\partial\psi_s}{\partial t}. \quad (3.3.4)$$

Now putting the value of $(E\psi_s)$ from (3.3.4) into (3.3.3) we get the following Schrödinger equation for a free particle

$$i\hbar\frac{\partial\psi_s}{\partial t} = \frac{-\hbar^2}{2m_0}\frac{\partial^2\psi_s}{\partial x^2}. \quad (3.3.5)$$

Differentiating $E\psi_s$, get

$$(p^2\psi_s) = -\hbar^2\frac{\partial^2\psi_s}{\partial x^2} . \quad (3.3.6)$$

Putting the both values of $(E\psi_s)$ and $(p^2\psi_s)$ into (3.3.5) we get

$$(E\psi_s) = \frac{p^2\psi_s}{2m_0} . \quad (3.3.7)$$

A particle in electromagnetic field with charge e placed, replacing E with $E - eV$ and p with $p - eA$ where V is scalar and A is a vector potential. Here $U = eV$ is potential energy. We know that the wave function is non-localized and it have a same values of E and p for all x and t . To obtain the required equation we need to consider a hypothetical case of U being constant.

For $v \ll c$, the magnetic field will be small and A can be neglected:

$$(E - U)\psi_s = \frac{1}{2m_0}(p - eA)^2\psi_s \cong \frac{p^2\psi_s}{2m_0}. \quad (3.3.8)$$

For simplicity we replace ψ_s by ψ and replace E and p by operators to get the Schrödinger equation.

$$i\hbar\frac{\partial\psi}{\partial t} = \frac{-\hbar^2}{2m_0}\frac{\partial^2\psi}{\partial x^2} + U\psi. \quad (3.3.9)$$

The related classical mechanics the total energy equation is

$$E = \frac{p^2}{2m_0} + U. \quad (3.3.10)$$

3.4 Corresponding principle between quantum and classical mechanics

Compare the quantum mechanical Schrödinger equation and classical mechanics energy equation. Write the corresponding between operators in quantum mechanics and variables in classical mechanical equation.

For $v \ll c$ we can write as $m_0 \cong m,$

Correspondence method: Following are the steps to convert a classical equation to quantum equation

1. Write the classical energy equation with energy E and momentum p as variables.
2. Multiply by a scalar wave function ψ on both sides.
3. To obtain the quantum equation replace E and p variables by corresponding operators.
4. Use reserve method to get a classical equation from mechanical equation.

Based on this method we get the following Klein- Gordon equation:
The classical energy equation is

$$E^2 = m_0^2 c^4 + p^2 c^2 \tag{3.4.1}$$

Apply condition 2 that multiply by ψ on both sides

$$\psi E^2 = m_0^2 c^4 \psi + p^2 c^2 \psi. \tag{3.4.2}$$

Replacing variables by operators

$$p^2 \iff p_{op}^2 = -\hbar^2 \frac{\partial^2}{\partial x^2}. \tag{3.4.3}$$

$$E^2 \iff E_{op}^2 = -\hbar^2 \frac{\partial^2}{\partial x^2}. \tag{3.4.5}$$

The quantum mechanical Klein-Gordon equation for a free particle reads

$$-\hbar^2 \frac{\partial^2 \psi}{\partial t^2} = m_0^2 c^4 (\psi) - \hbar^2 c^2 \frac{\partial^2 \psi}{\partial x^2}. \tag{3.4.5}$$

For a free we can write as

$$(\psi) = \frac{-\hbar^2}{p^2} \frac{\partial^2 \psi}{\partial x^2} = \frac{-\hbar^2}{\gamma^2 m_0^2 v^2} \frac{\partial^2 \psi}{\partial x^2}. \tag{3.4.6}$$

Put the value of (ψ) in Klein-Gordon equation and solve to obtain the wave equation

$$\frac{\partial^2 \psi}{\partial x^2} = \frac{1}{v_p^2} \frac{\partial^2 \psi}{\partial t^2}. \tag{3.4.7}$$

From above note that the wave equation is same as the Klein-Gordon equation .For $v \ll c$ we obtain quantum mechanical Schrödinger equation from this equation and the corresponding classical equation we get $E = \frac{p^2}{2m}$. Using the quantum energy and momentum operators

$$\frac{\partial^2 \psi}{\partial x^2} = \frac{p_{op}^2 \psi}{-\hbar^2} \tag{3.4.8}$$

$$\frac{\partial^2 \psi}{\partial t^2} = \frac{E_{op}^2 \psi}{-\hbar^2}. \tag{3.4.9}$$

Put above values in wave equation to write

$$E_{op}^2 \psi = v_p^2 p_{op}^2 \psi. \tag{3.4.10}$$

Cancel ψ and replace operators by variables. Substitute v_p and $E = mc^2$. the equation which is obtained by reverse method is a classical energy equation.

We observe that the wave equation is the base of all quantum mechanics equations and we can get the Klein-Gordon, Schrödinger equation and Dirac equation from it.

3.5 Schrödinger equation in spherical coordinates by correspondence method

The classical energy equation is

$$E = \frac{1}{2m}\left(\hat{n}p_r + \frac{\hat{l}}{r}p_\theta + \frac{\hat{m}}{rsin\theta}p_\emptyset\right).\left(\hat{n}p_r + \frac{\hat{l}}{r}p_\theta + \frac{\hat{m}}{rsin\theta}p_\emptyset\right) \tag{3.5.1}$$

where $\hat{n}, \hat{l}, \hat{m}$ are units vectors in $r, \theta, \emptyset$ direction

$$p_r = m\left(\frac{dr}{dt}\right) = m\left[\frac{dr}{dx}.\frac{dx}{dt} + \frac{dr}{dy}.\frac{dy}{dt} + \frac{dr}{dz}.\frac{dz}{dt}\right]. \tag{3.5.2}$$

Now we will use the correspondence method to write terms as below and to substitute in p_r.

$$m\left(\frac{dx}{dt}\right) = p_x \Leftrightarrow \frac{\hbar}{i}\frac{\partial}{\partial x}, \tag{3.5.3}$$

$$p_r \Leftrightarrow \frac{\hbar}{i}\left[\left(\frac{\partial r}{\partial x}\right)\frac{\partial}{\partial x} + \left(\frac{dr}{dy}\right)\frac{\partial}{\partial y} + \left(\frac{\partial r}{\partial z}\right)\frac{\partial}{\partial z}\right]. \tag{3.5.4}$$

From $x = rsin\theta cos\emptyset$ obtain terms such as $\frac{\partial r}{\partial x}$

$$\left(\frac{\partial}{\partial x}\right)_{yz} = \left(\frac{\partial r}{\partial x}\right)\frac{\partial}{\partial r} + \left(\frac{\partial \theta}{\partial x}\right)\frac{\partial}{\partial \theta} + \left(\frac{\partial \emptyset}{\partial x}\right)\frac{\partial}{\partial \emptyset} \tag{3.5.5}$$

$$\frac{\partial}{\partial x} = sin\theta cos\emptyset\frac{\partial}{\partial r} + \frac{cos\theta cos\emptyset}{r}\frac{\partial}{\partial \emptyset} - \frac{sin\emptyset}{rsin\theta}\frac{\partial}{\partial \emptyset}. \tag{3.5.6}$$

To obtain the operators p_θ and $p_\emptyset$ multiply by ψ in equation (3.5.1) and after multiplication replace all variables with related quantum operators:

$$E\psi = \frac{1}{2m}\left[\frac{\hbar}{i}\left(\hat{n}\frac{\partial}{\partial r} + \frac{\hat{l}}{r}\frac{\partial}{\partial \theta} + \frac{\hat{m}}{rsin\theta}\frac{\partial}{\partial \emptyset}\right).\frac{\hbar}{i}\left(\hat{n}\frac{\partial}{\partial r} + \frac{\hat{l}}{r}\frac{\partial}{\partial \theta} + \frac{\hat{m}}{rsin\theta}\frac{\partial}{\partial \emptyset}\right)\right]\psi. \tag{3.5.7}$$

Now we will get the required terms

such as

$$\frac{\partial \hat{n}}{\partial \theta} = \hat{l}\ .$$

The above values will now be used when expanding the bracket of (3.5.7). Now we will expand bracket with one term as follows and apply the above value

$$\frac{\hat{l}}{r}\frac{\partial}{\partial \theta}\left(\hat{n}\frac{\partial}{\partial r}\right) = \frac{\hat{l}}{r}\left[\hat{n}\frac{\partial}{\partial \theta \partial r} + \frac{\partial \hat{n}}{\partial \theta}.\frac{\partial}{\partial r}\right] = \frac{1}{r}\frac{\partial}{\partial r}. \tag{3.5.8}$$

Similarly we can solve all remaining terms and the Schrödinger equation becomes

$$E\psi_{r\theta\emptyset} = \frac{-\hbar^2}{2m}\left(\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\frac{\partial^2}{\partial \theta^2} + \frac{cos\theta}{r^2 sin\theta}\frac{\partial}{\partial \theta} + \frac{1}{r^2 sin^2\theta}\frac{\partial^2}{\partial \emptyset^2}\right)\psi_{r\theta\emptyset}. \tag{3.5.9}$$

The classical momentum variables and corresponding operators are

$$\hat{n}p_r = \hat{n}m\left(\frac{dr}{dt}\right) \Leftrightarrow \hat{n}\frac{\hbar}{i}\frac{\partial}{\partial r}, \quad \hat{l}p_\theta = \hat{l}mr^2\left(\frac{d\theta}{dt}\right) \Leftrightarrow \hat{l}\frac{\hbar}{i}\frac{\partial}{\partial \theta}, \quad \widehat{m}p_\emptyset = \widehat{m}mr^2 sin^2\theta\left(\frac{d\emptyset}{dt}\right) \Leftrightarrow \widehat{m}\frac{\hbar}{i}\frac{\partial}{\partial \emptyset}.$$

Angular Momentum using corresponding method:

$$v = \hat{n}\left(\frac{dr}{dt}\right) + \hat{l}r\left(\frac{d\theta}{dt}\right) + \widehat{m}rsin\theta\left(\frac{d\emptyset}{dt}\right) \tag{3.5.10}$$

where v is the velocity (given)

$$L = m(r \times v) = mr^2\left[\widehat{m}\left(\frac{d\theta}{dt}\right) - \hat{l}sin\theta\left(\frac{d\emptyset}{dt}\right)\right] \tag{3.5.11}$$

$$L^2 = L.L = m^2r^4\left[\left(\widehat{m}\left(\frac{d\theta}{dt}\right) - \hat{l}sin\theta\left(\frac{d\emptyset}{dt}\right)\right).\left(\widehat{m}\left(\frac{d\theta}{dt}\right) - \hat{l}sin\theta\left(\frac{d\emptyset}{dt}\right)\right)\right]. \tag{3.5.12}$$

Corresponding method (Multiply and replace variables by operators) we get

$$L^2\psi = m^2r^4\left[\left(\frac{\widehat{m}\hbar}{imr^2}\frac{\partial}{\partial\theta} - \frac{\hat{l}\hbar}{imr^2sin\theta}\frac{\partial}{\partial\emptyset}\right).\left(\frac{\widehat{m}\hbar}{imr^2}\frac{\partial}{\partial\theta} - \frac{\hat{l}\hbar}{imr^2sin\theta}\frac{\partial}{\partial\emptyset}\right)\right]\psi \tag{3.5.13}$$

$$L^2\psi = -\hbar^2\left(\frac{\partial^2}{\partial\theta^2} + \frac{cos\theta}{sin\theta}\frac{\partial}{\partial\theta} + \frac{1}{sin\theta^2}\frac{\partial^2}{\partial\emptyset^2}\right)\psi. \tag{3.5.14}$$

Note: L is a vector and is hard to compute if the direction is change and L2 is a scalar and easy to measure if its direction not dependent.

3.6 Schrödinger equation where potential energy $\mathrm{U(x)}$ is a function of x

The total energy remains constant all the time its trajectory for a particle in stable energy state, i.e. $E(x) = E_c$ for all$x$, describing the trajectory. The classical energy equation is

$$E_c = E(x) = \frac{p^2(x)}{2m} + U(x). \tag{3.6.1}$$

Here $U(x)$ is the function of x at position $x = x_n$ and $U(x_n) = U_n$.

I. Significance of the separation of variables

Classical energy equation of a particle at position $x = x_n$ and time $t = t_n$ is

$$E_n = E(x_n) = \frac{p^2(x_n)}{2m} + U(x_n) = \frac{p_n^2}{2m} + U_n. \tag{3.6.2}$$

Assume that there is a uniform potential $U(x_n) = U_n$ all over the space and write down the corresponding quantum mechanical Schrödinger equation as

$$-\frac{\hbar}{i}\frac{\partial\psi_n(x,t)}{\partial t} = -\frac{\frac{\hbar^2}{2m}\partial^2\psi_n(x,t)}{\partial x^2} + U(x_n)\psi_n(x,t). \tag{3.6.3}$$

The wave function is

$$\psi_n(x,t) = e^{-\frac{i}{\hbar}(E_nt - p_nx)}\ . \tag{3.6.4}$$

This is non-localized wave function which give the same value of momentum p_n for all x including at x_n . We can say that there is not anything incorrect as the corresponding principles requires that both the classical and quantum energy equation present similar energy and its true where the particle is placed i.e. at x_n.It means that even if the energy and momentum for a classical mass particle can be obtained mathematically for all values of x i.e. from$-\infty\ to + \infty$. Note that this wave function (non localized) do not give any information about the location of the classical particle in space.

By using the separation of variable method

$$\psi_n(x,t) = \varphi_n(x)T_n(t)$$

$$-\frac{\hbar}{iT_n(t)}\frac{\partial T_n(t)}{\partial t} = \frac{1}{\varphi_n(x)}\left(-\frac{\hbar^2}{2m}\frac{\partial^2\varphi_n(x)}{\partial x^2} + U(x_n)\varphi_n(x)\right) = E_n\ . \tag{3.6.5}$$

By using the above equation the time dependent part and time independent part can be separate. The separation of variables is acceptable in studying the wave function with respect to changes in x and t independently. A moving particle and its position is plotted in space independently with time t and the position will be similar to having a large number of particles in space at different locations on the trajectory of the particle. Note that the trajectory of the particle is determined by the nature of the potential field experienced by the particle.

II. Probability density

The wave of (3.6.3) is given by

$$\psi_n(x,t) = A(x,t) + iB(x,t) = A + iB \tag{3.6.6}$$

$$-\frac{\hbar}{i}\left(\frac{\partial A}{\partial t} + i\frac{\partial B}{\partial t}\right) = -\frac{\hbar^2}{2m}\left(\frac{\partial^2 A}{\partial x^2} + i\frac{\partial^2 B}{\partial x^2}\right) + U(x_n)(A + iB). \tag{3.6.7}$$

Separate real and imaginary parts and solve

$$\frac{\partial}{\partial t}(A^2 + B^2) = \frac{\hbar}{m}\frac{\partial}{\partial x}\left(B\frac{\partial A}{\partial x} - A\frac{\partial B}{\partial x}\right). \tag{3.6.8}$$

From above note that all terms are real. Compare with present equation

$$\frac{\partial\rho}{\partial t} = -\nabla.J \tag{3.6.9}$$

where the density is

$$\rho = A^2 + B^2 = \psi_n^*\psi_n\ . \tag{3.6.10}$$

The density is obtain as

$$J = \frac{\hbar}{m}\left(A\frac{\partial B}{\partial x} - B\frac{\partial A}{\partial x}\right) = \frac{\hbar}{2mi}\left[\psi_n^*(\nabla\psi_n) - (\nabla{\psi^*}_n)\psi_n\right]. \tag{3.6.11}$$

Momentum for the particle

$$p(x)(A + iB) = \frac{\hbar}{i}\frac{\partial}{\partial x}(A + iB), \tag{3.6.12}$$

$$p(x) = \frac{\hbar}{i}\frac{\left(\frac{\partial A}{\partial x}+\frac{i\partial B}{\partial x}\right)(A-iB)}{(A+iB)(A-iB)} = p_R + ip_I, \tag{3.6.13}$$

where $p_R = \hbar\frac{\left(A\frac{\partial B}{\partial x}-B\frac{i\partial A}{\partial x}\right)}{(A^2+B^2\ )}$.

Here p_R is real and p_I is imaginary component of momentum. We get this momentum for a single particle. If particles move in a varying potential field with mass, then the potential will vary with its position in space. Suppose that we have a system with a large number of particles each of mass m and density $\rho(x_n)$ at position x_n.Suppose also that the velocity in direction$X$ is $V_R(x_n)$ and that the Current per unit area is $J(x_n)$.We have

$$\frac{J(x_n)}{\rho(x_n)} = \frac{mV_R(x_n)}{m} = \frac{p_R}{m} = \frac{\frac{\hbar}{m}\left(A\frac{\partial B}{\partial x} - B\frac{\partial A}{\partial x}\right)}{A^2+B^2}. \tag{3.6.14}$$

As in (3.6.13), comparing numerator and denominator we get we get $J(x_n)$ and $\rho(x_n)$ .we can write for any $x = x_n$

$$\rho(x_n)V_R(x_n) = J(x_n) \tag{3.6.15}$$

Comparing 3.6.14) and (3.6.15) with classical current equations we write density of particles ρ as $\psi^*\psi$. For a single particle ρ is the density of resulting the particle in given unit volume at a exacting position which is called as the probability density.

So the concept of probability density we have found above only by similarity between the quantum equations and classical current equations. This step is difficult to explain in physical significance for a single particle.

III. Schrödinger equation for a varying potential

According to time independent:

Consider a system of larger number of particle and each particle have mass m at different positions such as $x_1, x_2 \dots x_n$ in space, placed in a potential field which is a function of x. The classical energy equation and corresponding quantum equation for a particle at x_n is written as

$$E_n = E_n(x) = \frac{p^2(x_n)}{2m} + U(x_n) = \frac{p_n^2}{2m} + U_n, \tag{3.6.16}$$

$$E_n\varphi_n(x) = -\frac{\hbar^2}{2m}\frac{\partial^2\varphi_n(x)}{\partial x^2} + U_n\varphi_n(x). \tag{3.6.17}$$

In single dimensional analysis, for small differential volume Δx at x_n, number of particles will be $\varphi_n^*(x_n)\varphi_n(x_n)\Delta x$. the total energy of particles at position x_n is $\varphi_n^*(x_n)E_n\varphi_n(x_n)\Delta x$. Average energy of all the particles in the system is

$$E_{av} = \frac{\varphi_1^*(x_1)E_1\varphi_1(x_1)\Delta x + \dots + \varphi_n^*(x_n)E_n\varphi_n(x_n)\Delta x}{\varphi_1^*(x_1)\varphi_1(x_1)\Delta x + \dots + \varphi_n^*(x_n)\varphi_n(x_n)\Delta x}. \tag{3.6.18}$$

Note that $E_1, E_2, \dots . E_n$ and $U_1, U_2, \dots, U_n$ are real quantities and we can write for all n,

$$\varphi_n^*(x_n)\varphi_n(x_n) = 1. \tag{3.6.19}$$

Now putting the required values in above equation from (3.6.17) as

$$E_{av} = \frac{\left[\varphi_1^*(x)\left(-\frac{\hbar^2}{2m}\frac{\partial^2\varphi_1(x)}{\partial x^2}\right)\right]_{x=x_1}\Delta x + \dots + \left[\varphi_n^*(x)\left(-\frac{\hbar^2}{2m}\frac{\partial^2\varphi_n(x)}{\partial x^2}\right)\right]_{x=x_n}\Delta x}{\varphi_1^*(x_1)\varphi_1(x_1)\Delta x + \dots + \varphi_n^*(x_n)\varphi_n(x_n)\Delta x}$$

$$+ \frac{\varphi_1^*(x_1)U_1\varphi_1(x_1)\Delta x + \dots + \varphi_n^*(x_n)U_n\varphi_n(x_n)\Delta x}{\varphi_1^*(x_1)\varphi_1(x_1)\Delta x + \dots + \varphi_n^*(x_n)\varphi_n(x_n)\Delta x}. \tag{3.6.20}$$

Canceling the denominator, by equating the above value of E_{av} with (3.6.18) ,

$$\sum_{i=1}^{n} E_i \Delta x = \sum_{i=1}^{n} \left[\varphi_i^*(x)\left(-\frac{\hbar^2}{2m}\frac{\partial^2 \varphi_i(x)}{\partial x^2}\right)\right]_{x=x_i} \Delta x + \sum_{i=1}^{n} U_i \Delta x. \tag{3.6.21}$$

Now we will define a new system wave function $\emptyset(x)$ such that for any position x_i ,

$$\left[\frac{1}{\varphi_i(x)}\left(-\frac{\hbar^2}{2m}\frac{\partial^2 \varphi_i(x)}{\partial x^2}\right)\right]_{x=x_i} = \frac{p_i^2}{2m} = \left[\frac{1}{\emptyset(x)}\left(-\frac{\hbar^2}{2m}\frac{\partial^2 \emptyset(x)}{\partial x^2}\right)\right]_{x=x_i}, \tag{3.6.22}$$

$$\sum_{i=1}^{n}[E(x)]_{x=x_i}\Delta x = \sum_{i=1}^{n}\left[\frac{1}{\emptyset(x)}\left(-\frac{\hbar^2}{2m}\frac{\partial^2 \emptyset(x)}{\partial x^2}\right)\right]_{x=x_i}\Delta x + \sum_{i=1}^{n}[U(x)]_{x=x_i}\Delta x. \tag{3.6.23}$$

A free particle can be travel at any location from $-\infty$ to $+\infty$ along X axis. The classical particle under influence of potential can oscillate between position x_1 and x_n .

In our system with large number of particles, the classical particles will be in the region $x_1 < x < x_n$. writing the equation in integration form

$$\int_{x_1}^{x_n} E(x)dx =$$

$$\int_{x_1}^{x_n}\left[\frac{1}{\emptyset(x)}\left(-\frac{\hbar^2}{2m}\frac{\partial^2 \emptyset(x)}{\partial x^2}\right)\right]dx + \int_{x_1}^{x_n} U(x)dx = \int_{x_1}^{x_n}\left(-\frac{\hbar^2}{2m\emptyset(x)}\frac{\partial^2 \emptyset(x)}{\partial x^2} + U(x)\right)dx. \tag{3.6.24}$$

A classical particle for stable state should have total energy $E(x) = E_C$ for all x between x_1 and x_n. As we see previous that if the particle is at a particular location x_i, the associated wave function has non-localized presence for all x from $-\infty$ to $+\infty$, we obtain

$$E_C = -\frac{\hbar^2}{2m\emptyset(x)}\frac{\partial^2 \emptyset(x)}{\partial x^2} + U(x)$$

$$E_C = \frac{1}{\emptyset(x)}\left(-\frac{\hbar^2}{2m}\frac{\partial^2 \emptyset(x)}{\partial x^2}\right) + U(x)) \tag{3.6.25}$$

$$E_C\emptyset(x) = -\frac{\hbar^2}{2m}\frac{\partial^2 \emptyset(x)}{\partial x^2} + U(x)\emptyset(x). \tag{3.6.26}$$

To obtaining a quantum equation corresponding classical equation, we will take help from probability density concept:

$$E_C = \frac{p^2(x)}{2m} + U(x). \tag{3.6.27}$$

According to time dependent:

E_n is energy at time t_n the particle is at x_n

$$-\frac{\hbar}{i}\frac{\partial T_n(t)}{\partial t} = E_n T_n(t), \tag{3.6.28}$$

$$[E_n]_{t=t_n} = \left[-\frac{\hbar}{i}T_n^*(t)\frac{\partial T_n(t)}{\partial t}\right]_{t=t_n}. \tag{3.6.29}$$

The average of all the n particles will be

$$\mathrm{E_{av}} = \frac{[\mathrm{E_1}]_{\mathrm{t=t_1}} + [\mathrm{E_2}]_{\mathrm{t=t_2}} + \cdots + [\mathrm{E_n}]_{\mathrm{t=t_n}}}{\mathrm{n}}. \tag{3.6.30}$$

For constant value of E_C for time requires

$$T_{1(t)} = T_{2(t)} = \cdots = T_{n(t)} = T(t)$$

so the value of the E_{av} will be for all values of time

$$E_{av} = E_C = n(-\frac{\hbar}{i}T^*(t)\frac{\partial T(t)}{\partial t}) \quad (3.6.31)$$

$$E_C = -\frac{\hbar}{i}\frac{1}{T(t)}\frac{\partial T(t)}{\partial t}. \quad (3.6.32)$$

Now we can get the Schrödinger equation by equating (3.6.32) and (3.6.25) and multiplying by $\psi(x,t) = \phi(x)T(t)$ where $U(x)$ is the potential energy of x.

$$-\frac{\hbar}{i}\frac{\partial\psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi(x,t)}{\partial x^2} + U(x)\psi(x,t) = E_{op}\psi(x,t) = E_C\psi(x,t). \quad (3.6.33)$$

All the constant values E_{C1}, E_{C2} ... corresponding to eigenfunctions ψ_1, ψ_2 ... will be eigenvalues of this equation and also the corresponding classical particle is in stable energy state. For a free particle the non localized wave function does not show the location of the classical particle. The probability density only offers a comparative picture of possible locations of the particle. From this equation can not get exact boundaries of oscillation x_1 and x_n of the classical particle. We can also say that the exact trajectory of a particle in space cannot obtain. The system wave function $\psi(x,t)$ can be described in form which is of a general nature

$$\psi(x,t) = A(x,t) + iB(x,t).$$

This $\psi(x,t)$ satisfies the Schrödinger equation .It can be used to analysis of probability density to obtain average value. The value of classical variable momentum can be mathematically obtained as

$$p(x) = \frac{\hbar}{i\psi(x)}\frac{\partial\psi(x)}{\partial x}. \quad (3.6.34)$$

Although from non-localized wave function we can get values of momentum for all x from $-\infty$ to $+\infty$. Typically also only the Hamiltonian (energy equation) does not give trajectory of the particle but it is balance of forces relation which decides shape of the orbit. Note that the quantum equations are energy equations and energy of a system is not localized.

3.7 Interpreting results of Schrödinger equation

I. Expectation values and measurement of a classical variable

The average value of energy by using probability density analysis for a normalized wave function is

$$E_{av} =< E >= \int \psi^*(x)E(x)\psi(x)dx.$$

For simplicity we will take one dimensional problem. If $\psi(x)$ is an eigenfuncion the $(x) = E_C$. According to corresponding method

$$E_C\psi(x) = E_{op}\psi(x)$$

$$E_{av} = \int \psi^*(x)E_{op}\psi(x)dx.$$

The eigenvalues will be same as average values for eigenfunctions. Quantities E and L^2 are scalar.

Suppose in given volume there are n particles with momentum$p_1\widehat{n_1}\,, p_2\widehat{n_2}\ , \dots , p_n\widehat{n_n}$.

There are two possibilities which are

Case 1. Let $p_1 = \cdots = p_n \neq 0$. If directions are such that

$$\widehat{n_1}\,,\widehat{n_2}\ , \dots , \widehat{n_n} = 0\ .$$

The average will be $p_{av} = 0$. For single particle if direction of motion changes incessantly and momentum is calculated at different time to find average value.

Case 2. Let $p_1 \neq \cdots \neq p_n$ and if direction is same then$\widehat{n_1} = \widehat{n_2}\ , \dots , = \widehat{n_n} = \hat{n}$.

Then average $p_{av} = \frac{1}{n}\hat{n}(p_1 + \cdots + p_n)$.

Note that if the direction of vector quantity does not be different then the direction of measurement can be associated with the direction of variable making measurement possible.

II. Hermitian property and energy operator

For $\psi(x)$, we find $p(x) = p_R + ip_I$. Energy expression $E(x) = \frac{p^2(x)}{2m}$ gives complex values. The following energy expression can give real value

$$E(x) = \frac{p^*(x)p(x)}{2m} = \frac{p_R^2 + p_I^2}{2m}\ .$$

But we cannot use $E = \frac{p^*p}{2m}$ in the correspondence principle as operator p_{op} acts on ψ and p_{op}^* acts on ψ^*. Momentum operator is Hermitian.

$$< \psi_1/p_{op}\psi_n \quad > = < p_{op}\psi_1/\ \psi_n >.$$

We know that the energy operator

$$E_{av} = \int_{-\infty}^{\infty} \psi^*(x)E_{op}\,\psi(x)dx = \int_{-\infty}^{\infty} \psi^*(x)\frac{p_{op}^2}{2m}\psi(x)dx = \int_{-\infty}^{\infty} \psi^*(x)\left(-\frac{\hbar^2}{2m}\frac{\partial^2\psi(x)}{\partial x^2}\right)dx$$

$$= -\frac{\hbar^2}{2m}\int_{-\infty}^{\infty} \psi^*(x)\left(\frac{\partial^2\psi(x)}{\partial x^2}\right)dx.$$

Define $\psi(x)$ as $\psi_n(x)$ and define $\psi^*(x)$ as $\psi_l^*(x)$ .choose $\psi(x)$ such that , $\psi(x)$ and $\psi^*(x) \to 0$ at $x \to \pm\infty$. integrate by parts

$$E_{av} = \frac{1}{2m}\int_{-\infty}^{\infty}\left(-\frac{\hbar}{i}\frac{\partial\psi_1^*(x)}{\partial x}\right)\left(\frac{\hbar}{i}\frac{\partial\psi_n(x)}{\partial x}\right)\,dx = \frac{1}{2m}\int_{-\infty}^{\infty}\left(p_{op}^*\psi^*(x)\right)\left(p_{op}\psi(x)\right)dx\ .$$

So we can use $E(x) = p^*(x)p(x)/2m$ as $E_{op} = p_{op}^2/2m$ with E_{op} and p_{op}^2 operators acting on function $\psi(x)$ to compute the average value.

III. Schrödinger equation and trajectory of a particle in motion

For a single dimension analysis suppose that system of N particles spread in space .if $\psi(x)$ is eigenfunction , $E(x) = E_C$ and $E_C\psi(x) = E_{op}\psi(x)$. Average energy of all particles is

$E_{av} = < E > = \frac{1}{N}$(Total energy of all particles).

$$E_{av} = \frac{\int_{-\infty}^{\infty} \psi^*(x)E(x)\psi(x)dx}{\int_{-\infty}^{\infty} \psi^*(x)\psi(x)dx} = \frac{\int_{-\infty}^{\infty} \left[\psi^*(x)\left(-\frac{\hbar^2}{2m}\frac{\partial^2\psi(x)}{\partial x^2}\right) + \psi^*(x)U(x)\psi(x) \right]}{\int_{-\infty}^{\infty} \psi^*(x)\psi(x)dx} = E_C \, .$$

The corresponding classical energy equation is

$$E_{av} = \langle \frac{p^2}{2m} + U \rangle = \langle p^* . \frac{p}{2m} + U \rangle = \left(\frac{p^2}{2m_{av}}\right)_{av} + (U)_{av} \, . \qquad (3.7.1)$$

Suppose the N particles have momentum$p_1\widehat{n_1}, \dots, p_N\widehat{n_N}$.

$$p_{av} = \frac{1}{N}(p_1\widehat{n_1} + \cdots + p_N\widehat{n_N})$$

$$(p^2)_{av} = \frac{1}{N}(p_1^2 + \cdots p_N^2).$$

In special case where $p_1 = \cdots = p_N = p$ and $\widehat{n_1} = \cdots = \widehat{n_N} = \hat{n}$ then $p_{av} = p\hat{n}$

So $(p^2)_{av} = p^2$. It only for this case we find $(p^2)_{av} = p_{av}.p_{av}$

We can get p_{av} from E_{av} .and for other case we will get as

$$(p^2)_{av} \neq p_{av}.p_{av}.$$

4. Numerical solution of Schrödinger equation

Consider the eigenvalue problem

$$-\Delta u + cu = \lambda u \quad \text{in } \Omega, \tag{4.1}$$

$$u = 0 \text{ on } \partial\Omega.$$

Multiply (4.1) by a function $v \epsilon H_0^1(\Omega)$ and integrate over Ω .After integration by parts we obtain the weak formulation of (4.1).

Find $u \epsilon H_0^1(\Omega)$ and $\lambda \epsilon \mathbb{R}$ such that

$$\int_\Omega Du.Dvdx + \int_\Omega cuvdx = \int_\Omega \lambda uvdx \tag{4.2}$$

For all $v\epsilon H_0^1(\Omega)$.

Let $L = -\Delta + c$.

L is self-adjoint if c is positive and has an orthonormal basis of eigenfunctions $\{V_i\}_{i=1}^{\infty}$ and a corresponding sequence of eigenvalues $\{\lambda_i\}_{i=1}^{\infty}$, $0 < \lambda_1 < \lambda_2$ ...

<u>FEM for (4.1)</u>

Define a mesh $\tau_h \subseteq \Omega$

Let $V_h = \{v\epsilon C(\Omega): v/K_h$ linear, $v = 0$ on $\partial\Omega\}$, K_h being triangles in 2D and subintervals in 1D.

Ω is a convex polygon in 2D and an interval in 1D.

We choose a basis in V_h ,$\{\varphi_i\}_{i=1}^N$ so that $V_h = span\{\varphi_i\}_{i=1}^N$

Further we let

$$U_h = \sum_{i=1}^N \xi_i \varphi_i \tag{4.3}$$

Weak FEM formulation

Find $u_h \epsilon V_h$ and λ_h such that

$$\int_\Omega Du_h.Dvdx + \int_\Omega cu_h vdx = \int_\Omega \lambda_h u_h vdx \tag{4.4}$$

For all $v\epsilon V_h$.

If we insert (4.3) into (4.4) we get, with the choice $v = \varphi_j$,$j = 1, \ldots, N$;

$$\int_\Omega D\left(\sum_{i=1}^N \xi_i\varphi_i\right).D\varphi_j dx + \int_\Omega c\left(\sum_{i=1}^N \xi_i\varphi_i\right)\varphi_j dx = \int_\Omega \lambda_h\left(\sum_{i=1}^N \xi_i\varphi_i\right)\varphi_j dx$$

Interchanging integration and sum we can write this as

$$\sum \xi_i \int_\Omega \left[\mathrm{D}\varphi_\mathrm{i}.\mathrm{D}\varphi_\mathrm{j}\mathrm{dx} + \int_\Omega \mathrm{c}\varphi_\mathrm{i}.\varphi_\mathrm{j}\mathrm{dx} \right] = \lambda_\mathrm{h} \sum \xi_i \int_\Omega \varphi_i \varphi_\mathrm{j}\mathrm{dx}, \quad \mathrm{j} = 1, \dots \mathrm{N}.$$

(4.5)

Letting

$$\mathrm{A_{ij}} = \int_\Omega \mathrm{D}\varphi_\mathrm{i}.\mathrm{D}\varphi_\mathrm{j}\mathrm{dx}$$

$$Mc_{ij} = \int_\Omega \mathrm{c}\varphi_i\varphi_j \,\mathrm{dx}$$

$$M = \int_\Omega \varphi_i \varphi_\mathrm{j}\mathrm{dx}$$

$\xi = (\xi_1, \dots, \xi_N)$.

We can write (4.5) as

$$[A + Mc\,]\xi = \lambda_h \mathrm{M}\xi$$

Or equivalently

$$M^{-1}[A + Mc]\xi = \lambda_h \xi\ . \tag{4.6}$$

This is a matrix eigenvalue problem which can be solved via

$\lambda_h = \mathrm{eig}(\mathrm{M}^{-1}[\mathrm{A} + \mathrm{Mc}])$ in Matlab.

4.1 Error estimates

We have the following errors estimates for the computed eigenvalues and eigenfunctions

$0 \leq \lambda_\mathrm{h} - \lambda \leq \mathrm{c}\|\mathrm{hD}^2\mathrm{u}\|^2_{\mathrm{L}^2(\Omega)}$

$\|\mathrm{u} - \mathrm{u_h}\|_{\mathrm{L}^2(\Omega)} \leq \mathrm{c}\left(1 + \frac{2\lambda}{\mathrm{d}}\right) \left\|\mathrm{h}^2\mathrm{D}^2_\mathrm{h}\right\|_{\mathrm{L}^2(\Omega)}$

d being the distance between λ its closest neighbor eigenvalue, where (u, λ) is the eigen-couple associated to (4.1).

Let us now consider the Schrödinger equation for particle with mass m in a potential $\mathrm{V} = \mathrm{V}(\mathrm{x})$.

$$-\frac{\hbar^2}{2\mathrm{m}}\Delta\psi + \mathrm{V}\psi = \mathrm{i}\hbar\frac{\partial\psi}{\partial \mathrm{t}} \tag{4.7}$$

A Separation of variables:

$$\psi(x,t) = u(x)v(t)$$

leads to

$$-\frac{\hbar^2}{2m}\Delta u.v + Vuv = i\hbar\frac{\partial v}{\partial t}u . \qquad (4.8)$$

We divide by uv in (4.8)

$$-\frac{\hbar^2}{2mu}\Delta u. + V = \frac{i\hbar}{v}\frac{\partial v}{\partial t}(t) = E \qquad (4.9)$$

We obtain two equations as we discuss before in equation (2.2.1) and we find these two equations

$$-\frac{\hbar^2}{2m}\Delta u. + Vu = Eu \qquad (4.10)$$

$$i\hbar\frac{\partial v}{\partial t}(t) = Ev . \qquad (4.11)$$

Equation (4.10) is the eigenvalue problem for the time independent Schrödinger equation, and it is of the same types as (4.1). The quantity

$$H = -\frac{\hbar^2}{2mu}\Delta + V$$

is called the Schrödinger Hamiltonian.

4.2 Simulations of eigenvalues

For FEM-Computation in 1D

Example 1.

Consider the problem of finding values of λ such that

$$-u'' + x^2u = \lambda u \qquad [-8\ 8] \qquad (4.12)$$

$$u(-8) = u(8) = 0$$

This is the problem of a quantum harmonic oscillator in 1D, whose exact solution is

$$\lambda_1 = 1$$

$$\lambda_2 = 3$$

$$\lambda_3 = 5$$

$$\lambda_4 = 7$$

To approximate the eigenvalues of (4.12) we use a 1-dimensional FEM-program.

We perform simulations with uniform meshes on [-8, 8] with interval length *h=0.1, h=0.01 and h=0.001.*

We get the following results

h	λ_1	λ_2	λ_3	λ_4
0.1	1.0015	3.0040	5.0090	7.0164

h	λ_1	λ_2	λ_3	λ_4
0.01	1.0000	3.0000	5.0001	7.0002

2D problem

Example 2

Consider the eigenvalue problem in the plane

$$\begin{cases} -\Delta u = \lambda u & \text{on } \Omega \\ u = 0 & \text{on } \partial\,\Omega \end{cases} \tag{4.13}$$

Ω Unit circle entered at origin

We will calculate the six first eigenmodes of vibration of a drum (modeled as a circular membrane fixed at its boundary).we will use a finite element method. Now we will run the following file Eig1.m, Eig2.m and EigenSolver.m and we get the following result as shown in table 4.2.1

Eigenmode	1	2	3	4	5	6
Eigenvalue	5.8014	14.7883	14.7929	26.7330	26.7389	30.9336

Table 4.2.1 Eigenvalues corresponding to the eigenmodes of Figure 4.2.1

We note from the table that the first eigenvalue is simple while the second and the third are double.

We also notice that for a small potential we get essentially the same eigenvalues as for the case without potential.

It turns out that the correct scaling of the quantum oscillator is to choose the potential large compared to the Laplace term.

The so called semi classical asymptotes of the Schrödinger potential is the study of the limit of

$$-\Delta u_\varepsilon + \frac{1}{\varepsilon^2} V\left(\frac{x}{\varepsilon}\right) u_\varepsilon = \lambda_\varepsilon u_\varepsilon$$

As $\varepsilon \to 0$, where we assume that the potential $V\left(\frac{x}{\varepsilon}\right)$ is periodic with period$\varepsilon > 0$.

This limit has been studied by means of WKB-analysis and homogenization theory.

We will not consider this here, but we present in example 4, some computations where we increase the size of the potential.

Example3

Quantum harmonic oscillator in 2D

$$\begin{cases} -\Delta u + (x_1^2 + x_2^2)u = \lambda u \\ u = 0 \quad on\ \partial\Omega \end{cases} \text{ on } \Omega$$

We get the following numerical result

Ans =1.0e+02*

Eigenmode	1	2	3	4	5	6
Eigenvalue	0.6433	1.2957	1.2981	1.9570	1.9591	1.9727

Table 4.2.2 Eigenvalues corresponding to the eigenmodes of Figure 4.2.2

Example 4

Consider the eigenvalue problem

$$-\frac{\hbar^2}{2m}\Delta u + (x_1^2 + x_2^2)u = \lambda u$$

We compute the eigenvalues for very large potentials

i. $-\Delta u + 10^3(x_1^2 + x_2^2)u = \lambda u$
ii. $-\Delta u + 10^6(x_1^2 + x_2^2)u = \lambda u$
iii. $-\Delta u + 10^9(x_1^2 + x_2^2)u = \lambda u$

After running a standard finite element code in Matlab for above three problems we get the following results respectively

i. Ans =1.0e+02*

Eigenmode	1	2	3	4	5	6
Eigenvalue	0.6433	1.2957	1.2981	1.9570	1.9591	1.9727

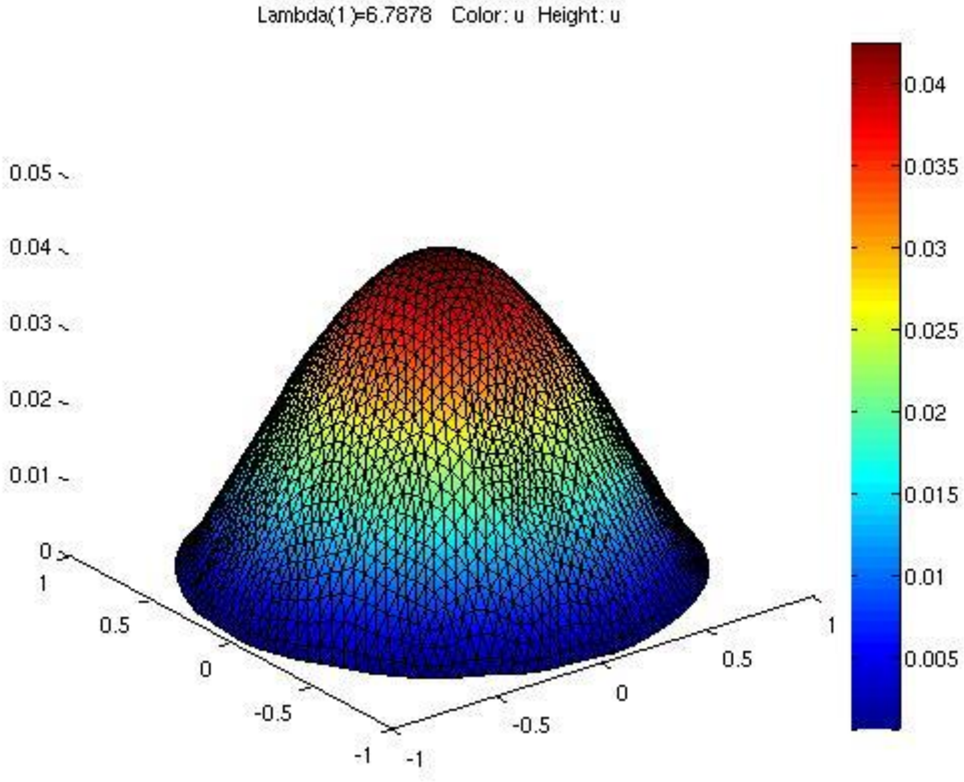
ii. Ans=1.0e+4*

Eigenmode	1	2	3	4	5	6
Eigenvalue	0.3852	0.8742	0.9980	1.3222	1.3722	1.8367

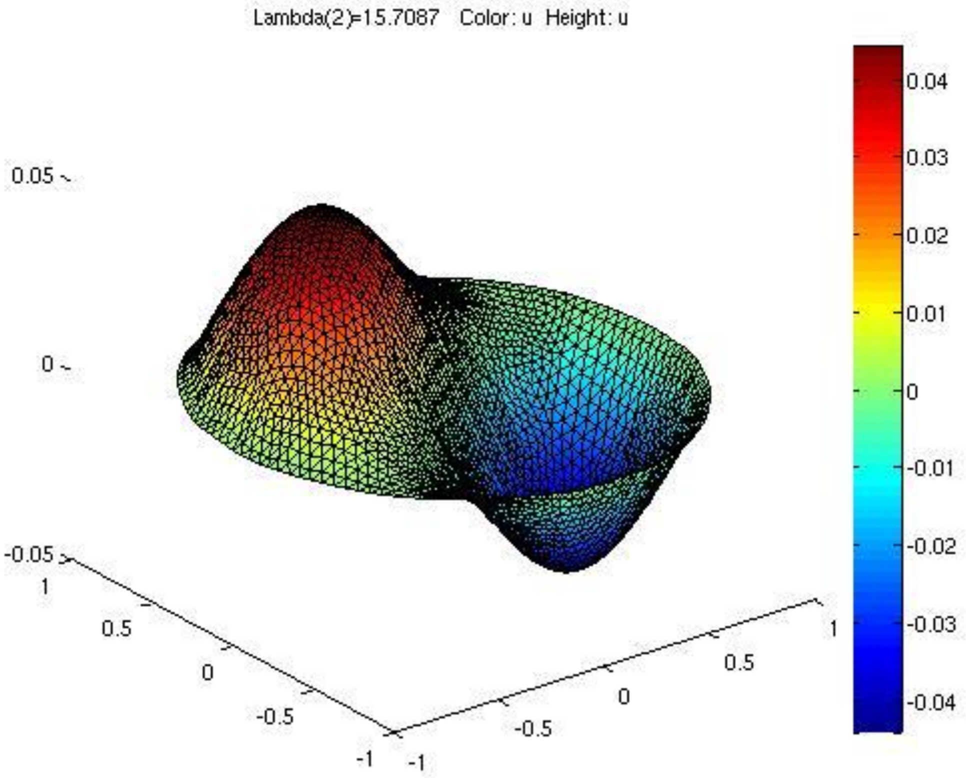
The eigenfunctions for the first five eigenvalues of the eigenvalue problem

$$\begin{cases} -\Delta u + \ ku = \lambda u \\ u = 0 \qquad \text{on } \partial\Omega \end{cases}$$

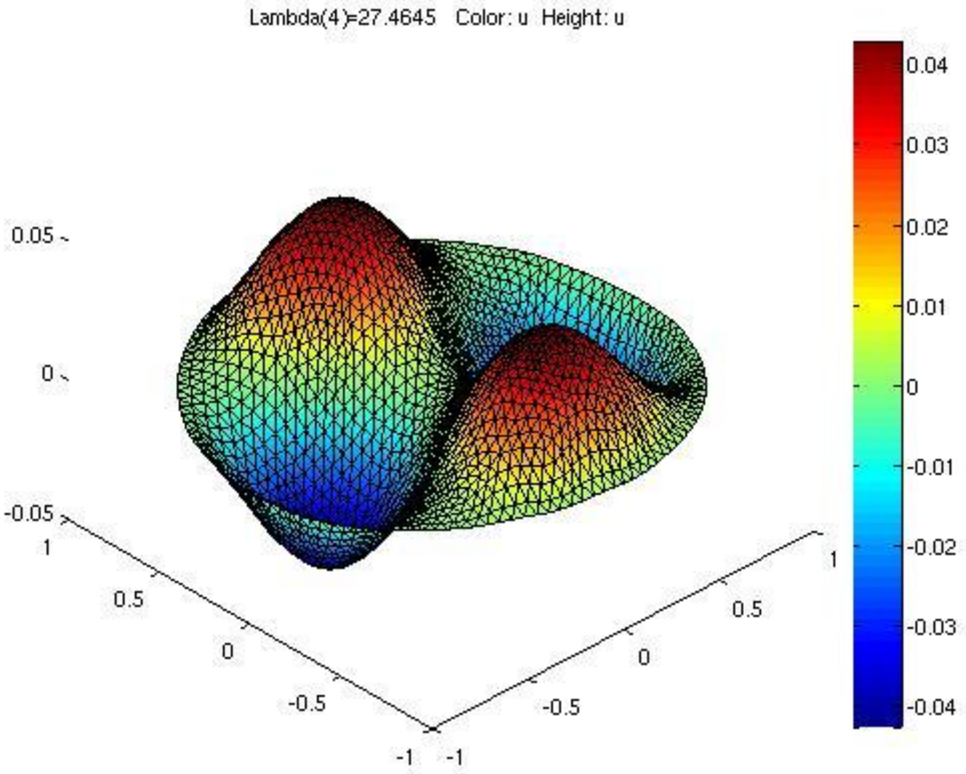
With k=1 are shown in Figure 1-5 below



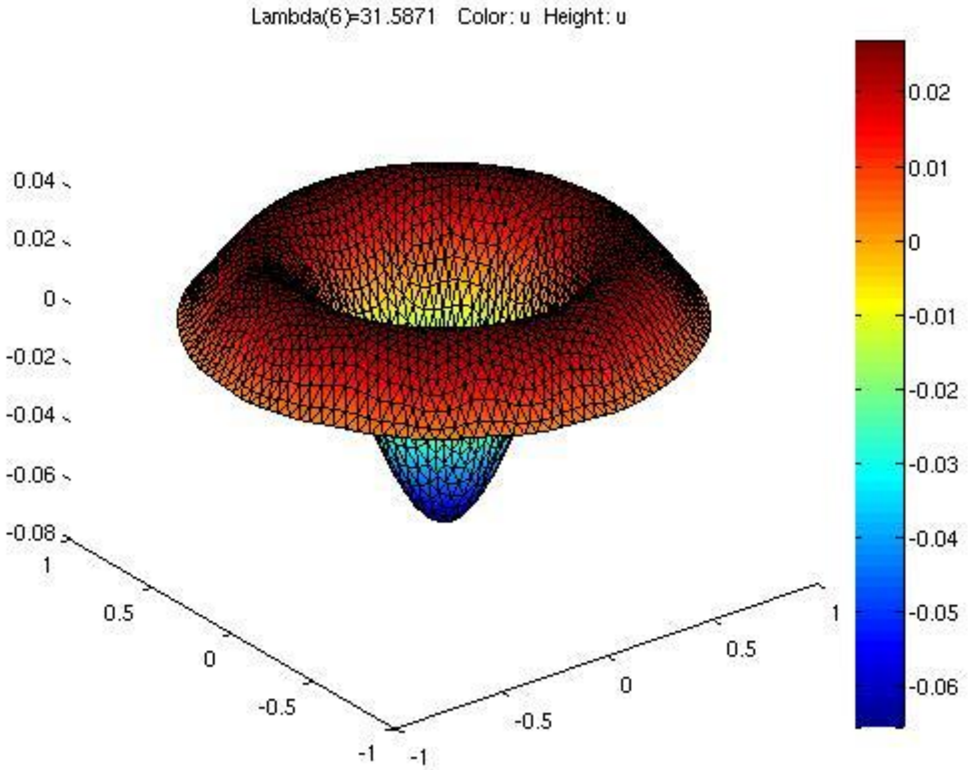
Figur 1



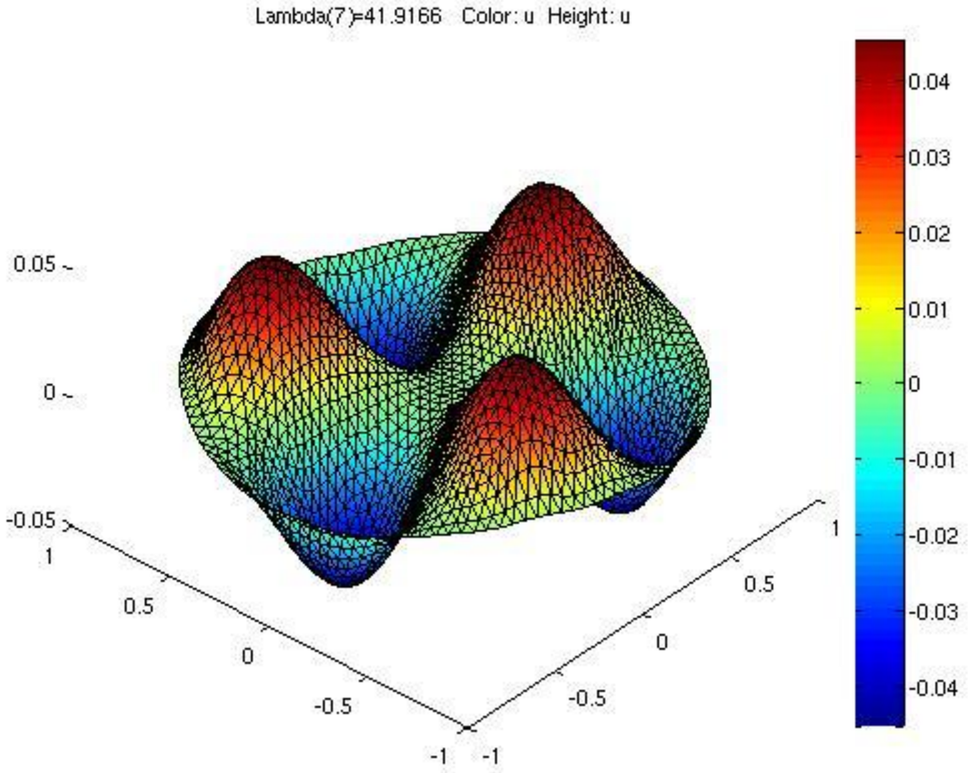
Figur 2



Figur 3



Figur 4



Figur 5

4.3 Spectral method

We will first consider the problem of computing derivatives numerically

Consider a set of grid points in $\mathbb{R}$ $\{x_j\}^N_{j=0}$ and a corresponding set of function values $\{u(x_j)\}$ for a given function : $\mathbb{R} \to \mathbb{R}$.

Let the grid be uniform with

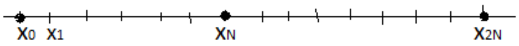
$$x_{j+1} - x_j = h \ , j = 0, \ldots., N-1.$$

The symmetric difference quotient

$w_j = \frac{u_{j+1} - u_{j-1}}{2n}.$

Is a common approximation to $u'(x_j)$.

Let us now assume that u is periodic with $u_0 = u_N \quad , u_1 = u_{N+1\ldots}$ where $\quad u_j = u(x_j)$.



We can express the ``derivatives' 'in matrix form

$$W = AU$$

where

$$W = \begin{pmatrix} w_1 \\ \vdots \\ w_N \end{pmatrix} , A_2 = \frac{1}{h} \begin{pmatrix} 0 & \frac{1}{2} & & -\frac{1}{2} \\ -\frac{1}{2} & \ddots & \ddots & \\ & \ddots & \ddots & \frac{1}{2} \\ \frac{1}{2} & & -\frac{1}{2} & 0 \end{pmatrix}$$

$$U = \begin{pmatrix} u_1 \\ \vdots \\ u_N \end{pmatrix}.$$

The matrix A is Toeplitz , i.e. has constant entries along diagonals. This method of approximating derivatives is of second order, and we call A a differentiation matrix.

For again a periodic function u a forth order differentiation matrix has the form

$$A_4 = \frac{1}{h}\begin{pmatrix} \ddots & & \ddots & \vdots & & \frac{1}{12} & -\frac{2}{3} \\ & & \ddots & -\frac{1}{3} & \ddots & & \frac{1}{12} \\ & & \ddots & -\frac{1}{2} & \ddots & & \\ & & \ddots & 1 & \ddots & & \\ & & \ddots & 0 & \ddots & & \\ & & \ddots & -1 & \ddots & & \\ & & \ddots & \frac{1}{2} & \ddots & \ddots & \\ -1/12 & & \ddots & -\frac{1}{3} & \ddots & & \ddots \\ 2/3 & -1/12 & & \vdots & & & \end{pmatrix}$$

The order of the matrix yields the convergence routes for smooth

$u\colon \mathbb{R} \to \mathbb{R}$

with A_2 $\quad w_j \to u'(x_j) \qquad O(h^2) \;\; as\; h \to 0$

with A_4 $\quad w_j \to u'(x_j) \qquad O(h^4) \;\; as\; h \to 0$

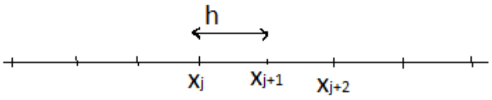
It can be shown that by increasing the order and the bandwidth one obtains the Laurent operator

A_L Which is a skew symmetric $[A_L^T = -A_L]$ doubly infinite Toeplitz matrix.

$$A_L = \frac{1}{h}\begin{pmatrix} \ddots & \vdots & \\ \ddots & -\frac{1}{3} & \ddots \\ \ddots & -\frac{1}{2} & \ddots \\ \ddots & 1 & \ddots \\ \ddots & 0 & \ddots \\ \ddots & -1 & \ddots \\ \ddots & \frac{1}{2} & \ddots \\ \ddots & -\frac{1}{3} & \ddots \\ & \vdots & \end{pmatrix}.$$

In practice one does not use infinite matrices, but we will use spectral truncated Laurent operators.

Let us now introduce an infinite grid $h\mathbb{Z}$ with grid points $x_j = jh$ for $\mathbb{Z}$:



We recall for $u\,\epsilon\mathbb{R}$ the Fourier transformation

$$\hat{u}(k) = \int_{-\infty}^{\infty} e^{-ikx}\, u(x)dx, \quad k\epsilon\mathbb{R}. \tag{4.3.1}$$

with inverse

$$u(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{ikx}\, \hat{u}(k)dx, \quad x\epsilon\mathbb{R}\ . \tag{4.3.2}$$

Let now $x\epsilon h\mathbb{Z}$, so that the values of x are uniformly distributed along the real axis with distance h .

As a consequence the wave number k will not range over $\mathbb{R}$, but on the bounded interval $[-\frac{\pi}{h},\frac{\pi}{h}]$ of length $\frac{2\pi}{h}$.

For a function v defined on $h\mathbb{Z}$ with $v_j = v(x_j)$ we defined the semi discrete Fourier transformation

$$\hat{u}(k) = h\sum_{j=-\infty}^{\infty} e^{-ikx_j}\, v(x_j), \qquad k\epsilon\left[-\frac{\pi}{h},\frac{\pi}{h}\right] \tag{4.3.3}$$

with inverse semi discrete Fourier transformation

$$v(x_j) = \frac{1}{2\pi}\int_{-\frac{\pi}{h}}^{\frac{\pi}{h}} e^{ikx_j}\, \hat{v}(k)dk, \quad j\epsilon\mathbb{Z}. \tag{4.3.4}$$

We see that (4.3.3) approximates (4.3.1) by the trapezoid rule and (4.3.4) approximates (4.3.2) by truncating $\mathbb{R}$ to $[-\frac{\pi}{h},\frac{\pi}{h}]$.

In order to define spectral differentiation we need an interpolant .we define

$$p(x) = \frac{1}{2\pi}\int_{-\frac{\pi}{h}}^{\frac{\pi}{h}} e^{ikx}\, \hat{v}(k)dk, \quad x\epsilon\mathbb{R}. \tag{4.3.5}$$

This function satisfies that

$p(x_j) = v(x_j)\,,\ j\epsilon\mathbb{Z}$ in addition p is analytic and

$$\hat{p}(k) = \begin{cases} \hat{v}(k), & k\epsilon\left[-\frac{\pi}{h},\frac{\pi}{h}\right]. \\ 0 & , \text{ otherwise.} \end{cases}$$

We call p the band limited interpolant of v.

Definition:

The spectral derivative of v is given as

$$w_j = p'(x_j)$$

where p is computed by (4.3.5).

This can also be phrased:

Given v compute the semi descrete Fourier transformation $\hat{v}$ in (4.3.3).

Define $\widehat{w}(k) = ik\hat{v}(k)$. compute w from $\widehat{w}$ using (4.3.4).

Using this we can derive the entries of A_L . Let

$$\delta_j = \delta(x_j) = \begin{cases} 1\,, & j = 0 \\ 0\,, & j \neq 0 \end{cases}$$

By (4.3.3) $\hat{\delta}(k) = h$ for all$k\epsilon\left[-\frac{\pi}{h},\frac{\pi}{h}\right]$. By (4.3.5) the band limited interplotant of δ is

$$p(x) = \frac{h}{2\pi}\int_{-\frac{\pi}{h}}^{\frac{\pi}{h}} e^{ikx}\,dx = \frac{\sin\left(\frac{\pi x}{h}\right)}{\frac{\pi x}{h}} = S_h(x).$$

We can now write

$$N(x_j) = \sum_{m=-\infty}^{\infty} v(x_m)\delta(x_{j-m})$$

for any v defined on $h\mathbb{Z}$.

Its band limited interpolant can then be written as

$$p(x) = \sum_{m=-\infty}^{\infty} v(x_m)S_h(x - x_m)$$

with derivatives

$$w_j = p'(x_j) = \sum_{m=-\infty}^{\infty} v(x_m) S_h'(x_j - x_m).$$

The entries of A_L are given by

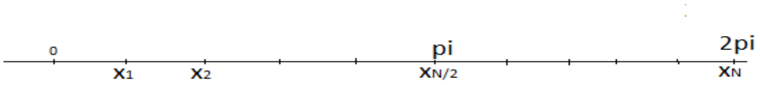
$$S_h'(x_j) = \begin{cases} 0\,, & j = 0 \\ \dfrac{(-1)^j}{j^h}\,, & j \neq 0. \end{cases}$$

For higher order derivatives we have the formula

$$S_h''(x_j) = \begin{cases} -\dfrac{\pi^2}{3h^2}\,, & j = 0 \\ \dfrac{2(-1)^{j+1}}{j^2 + h^2}\,, & J \neq 0 \end{cases}$$

$$B_L = \frac{2}{h^2}\begin{pmatrix} \ddots & \vdots & \\ \ddots & -\frac{1}{4} & \ddots \\ \ddots & -\frac{\pi^2}{6} & \ddots \\ \ddots & 1 & \ddots \\ \ddots & -\frac{1}{4} & \ddots \\ & \vdots & \ddots \end{pmatrix}.$$

Let us now return to periodic grids. Our basic grid will be $[0, 2\pi]$.



We assume N even and periodicity means

$$V(x_{j+mN}) = v(x_j) \qquad j, m \,\epsilon\, \mathbb{Z}$$

$$h = \frac{2\pi}{N} \qquad \text{or} \frac{\pi}{h} = \frac{N}{2}.$$

We recall that for discrete values $\{x_j\}$ the wave numbers k are bounded.Scince we require v to be periodic , k must be integer values by the inversion formula.

Discrete Fourier transformation DFT

$$\hat{v}(k) = h \sum_{j=1}^{N} e^{-ikx_j}\, v(x_j)\ , \quad k = -\frac{N}{2} + 1, \dots, \frac{N}{2}\ . \tag{4.3.6}$$

Inverse DFT

$$v(x_j) = h \sum_{k=-\frac{N}{2}+1}^{N/2} e^{ikx_j}\,\hat{v}(k) \ , \quad j = 1, \ldots, N. \tag{4.3.7}$$

The $N \times N$ spectral differentiation matrix D_N corresponding to the DFT of the band limited interpolant is given by

$$D_N = \begin{pmatrix} 0 & -\frac{1}{2}\cot\frac{h}{2} \\ -\frac{1}{2}\cot\frac{h}{2} & \frac{1}{2}\cot\frac{h}{2} \\ \frac{1}{2}\cot\frac{2h}{2} & \frac{1}{2}\cot\frac{h}{2} \\ -\frac{1}{2}\cot\frac{3h}{2} & \frac{1}{2}\cot\frac{h}{2} \\ \vdots & \vdots \\ \frac{1}{2}\cot\frac{h}{2} & 0 \end{pmatrix}.$$

The second order differentiation matrix is given by

$$D_N^{(2)} = \begin{pmatrix} \ddots & -\frac{1}{2}\csc^2\frac{2h}{2} & \\ \ddots & \frac{1}{2}\csc^2\frac{h}{2} & \ddots \\ \ddots & -\frac{\pi^2}{3h^2} - \frac{1}{6} & \ddots \\ & \frac{1}{2}\csc^2\frac{h}{2} & \ddots \end{pmatrix}.$$

Example 5

Let us now apply spectral method to the quantum harmonic oscillator

$$-u''(x) + x^2 u(x) = \lambda u(x) \ , \qquad x \epsilon \mathbb{R} \tag{4.3.8}$$

It is well-known that the exact eigenvalues are $\lambda = 1, 3, 5, \ldots$..

The eigenfunctions are Hermite polynomials $H_n(x)$ multiplied by exponentials $e^{-\frac{x^2}{2}}$, so we have eigenvalues

$0 < \lambda_1 < \lambda_2 < \lambda_3 <, \ldots,$ $\qquad \lambda_1 = 1, \lambda_2 = 3$ etc.

with eigenfunctions

$$\varphi_n(x) = e^{-\frac{x^2}{2}} H_n(x), \qquad n = 1, 2, \ldots.$$

Since the eigenfunctions decay rapidly we truncate the infinite spatial interval to the periodic interval $[-L, L]$, L is large enough. Let $\{x_j\}_{j=1}^{N}$ be a uniform grid in $[-L, L]$.

Let v be the approximation of the solution u to (4.3.8) at the grid points. The discrete approximation of (4.3.8) reads

$$(-D_N^2 + S)v = \lambda v \qquad (4.3.9)$$

where D_N^2 is the matrix above rescaled to $[-L, L]$. $S = diag(x_1^2 +, \ldots., x_N^2)$.

Hence the eigenvalues of (4.3.8) are approximated by those of (4.3.9).

Program 1

```
format long, format compact

L=8;

for N=6:6:36

  h=2*pi/N; x=h*(1:N); x=L*(x-pi)/pi;

  column=[-pi^2/(3*h^2)-1/6 ...

    -.5*(-1).^(1:N-1)./sin(h*(1:N-1)/2).^2];

  D2=(pi/L)^2*toeplitz(column); %2nd order differentiation

  eigenvalues=sort(eig(-D2+diag(x.^2)));

  N,eigenvalues(1:4)

end
```

We get the following results

N=6	N=12
0.461472916995476 7.494134621050528 7.720916053006555 28.832483778340144	0.978137281298606 3.171605320647186 4.455935291166786 8.924529058119928
N=18	N=24
0.999970001499310 3.000644066795823 4.992595324407715 7.039571897981499	0.999999997629044 3.000000098410865 4.999997965273282 7.000024998156531
N=30	N=36
1.000000000000003 3.000000000000729 4.999999999975589 7.000000000508604	0.999999999999992 2.999999999999944 4.999999999999982 7.000000000000007

Why the Spectral method works so well

Compare this with the FEM-computation in 1D, which is much slower and has much less accuracy.
The computing time with *N=36* in the spectral method is functions of a second, the computing time in Example 1 with interval length *h=0.001 is* function of more than 30 minutes.
Its remarkable that with N=36 the first 4 eigenvalues are computed with 13 correct digits using (4.9) .

The reason is that for smooth functions the Fourier transformation decays rapidly. So that aliasing errors due to discretization are small.

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