Chapter 23 ODE (Ordinary Differential Equation)

Speaker: Lung-Sheng Chien

Reference: [1] Veerle Ledoux, Study of Special Algorithms for solving Sturm-Liouville and Schrodinger Equations.

[2] 陳振臺, university physics, lecture 5

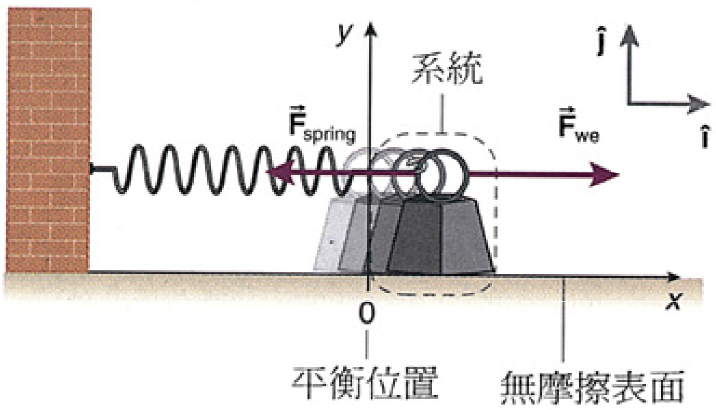
[3] Harris Benson, university physics, chapter 15

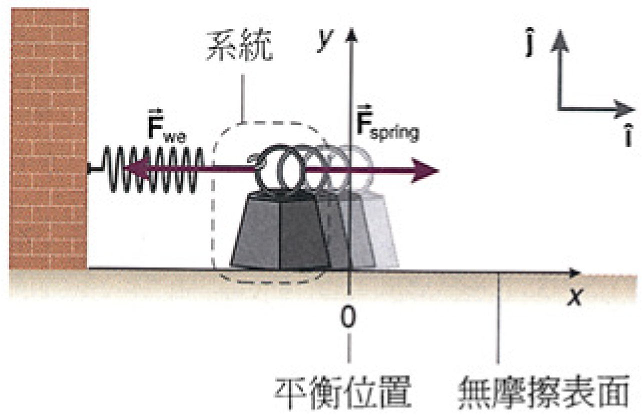
Hook's Law (虎克定律)　[1]

在水平方向作用於系統的力量有二(見下圖)：

$\vec{F}_{we}$：我們施於物體拉扯彈簧的力

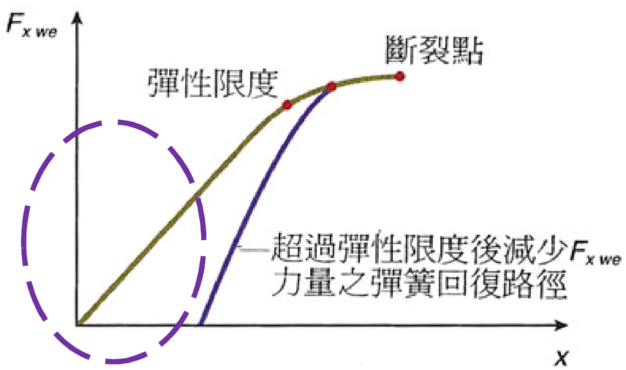
$\vec{F}_{spring}$：彈簧作用於物體的力





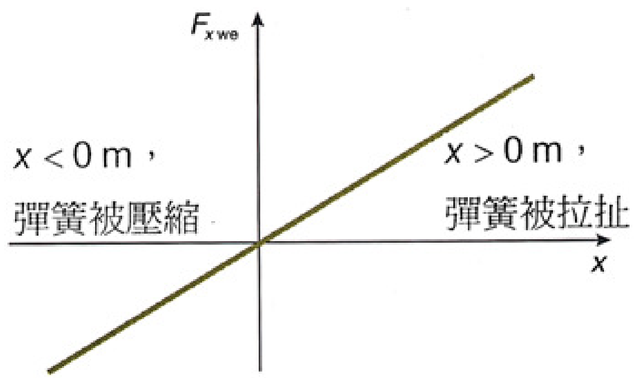
若我們施力在物體上來壓縮彈簧 (見上圖)，則彈簧作用於*m*的力量方向同樣地與我們的施力方向相反

彈簧作用於物體 (質量*m*)的力試圖將物體回復到平衡位置，無論彈簧是被拉扯或被壓縮，它的方向總是朝向平衡位置稱爲回復力，因爲其作用在將質量回復到平衡位置處。

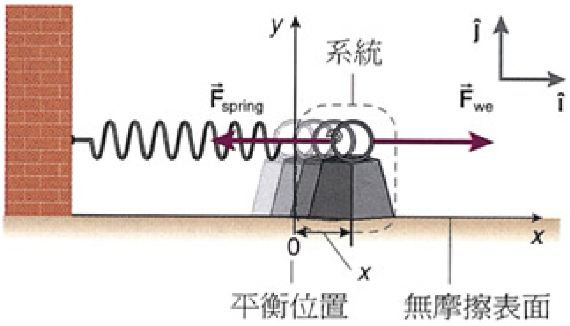


虎克定律: $\vec{F}_{we} = kx\ \hat{i}$

k：彈性係數和物體無關

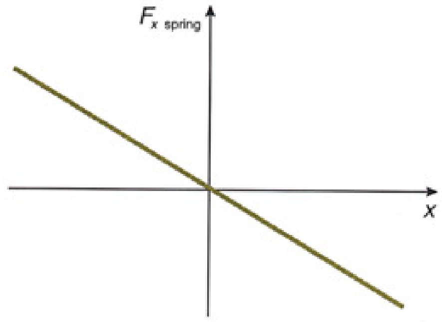


Hook’s Law (虎克定律)　[2]

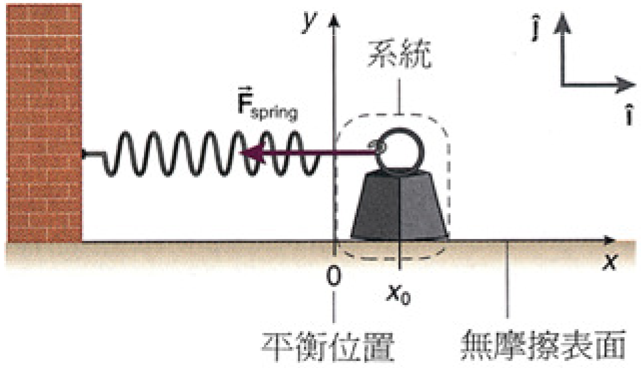


如左圖所示，物體被固定於x之位置

$$\begin{cases} \vec{F}_{spring} + \vec{F}_{we} = 0 \\ \vec{F}_{we} = kx\,\hat{i} \end{cases} \longrightarrow \vec{F}_{spring} = -kx\,\hat{i}$$



彈簧作用於m的力與彈簧被拉扯或被壓縮的量成正比，且方向總是朝向平衡位置



我們由一個物體m繫於一個理想彈簧上開始，而此系統為在水平無摩擦的表面上。我們將此質量向右拉一個距離為，然後在物體靜止時突然 (瞬間地) 釋放，如左圖所示。

當彈簧力為唯一作用於m的力量，且朝著一個指定的方向，此時m的振盪運動就是**簡諧振盪**，並且其排列被稱之為簡諧振子 (simple harmonic oscillator)。

牛頓第二運動定律: $\vec{F} = ma$ $\xrightarrow[\text{位移 } \vec{r} = x\,\hat{i},\ \vec{a} = \frac{d^2}{dt^2}\vec{r}]{\vec{F} = \vec{F}_{spring} = -kx\,\hat{i}}$ $m\dfrac{d^2x}{dt^2} = -kx$

$x > 0$: 平衡點右側

$x < 0$: 平衡點左側

Hook's Law (虎克定律) [3]

$$m\frac{d^2x}{dt^2} = -kx \longrightarrow \frac{d^2x}{dt^2} + \frac{k}{m}x = 0 \xrightarrow{\text{dimension analysis}} \left[\frac{d^2x}{dt^2}\right] = \frac{meter}{\sec^2}, \quad \left[\frac{k}{m}x\right] = \left[\frac{k}{m}\right] meter$$

We must match dimension of each term in the equation $\left[\frac{k}{m}\right] = \frac{1}{\sec^2} = 頻率^2$

Period (周期) $T = \frac{2\pi}{w}$

Definition: $w = \sqrt{\frac{k}{m}} \equiv 2\pi f$ 振盪的角頻率(angular frequency)，單位爲 rad/s

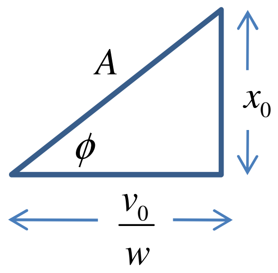
$$\frac{d^2x}{dt^2} + w^2 x = 0 \xrightarrow[x = \exp(\lambda t)]{\text{guess}} \begin{matrix}(\lambda^2 + w^2)x = 0 \\ \lambda = \pm iw\end{matrix} \longrightarrow \begin{matrix} x = Ae^{iwt} + Be^{-iwt} \quad \text{or} \\ x = C\cos(wt) + D\sin(wt)\end{matrix}$$

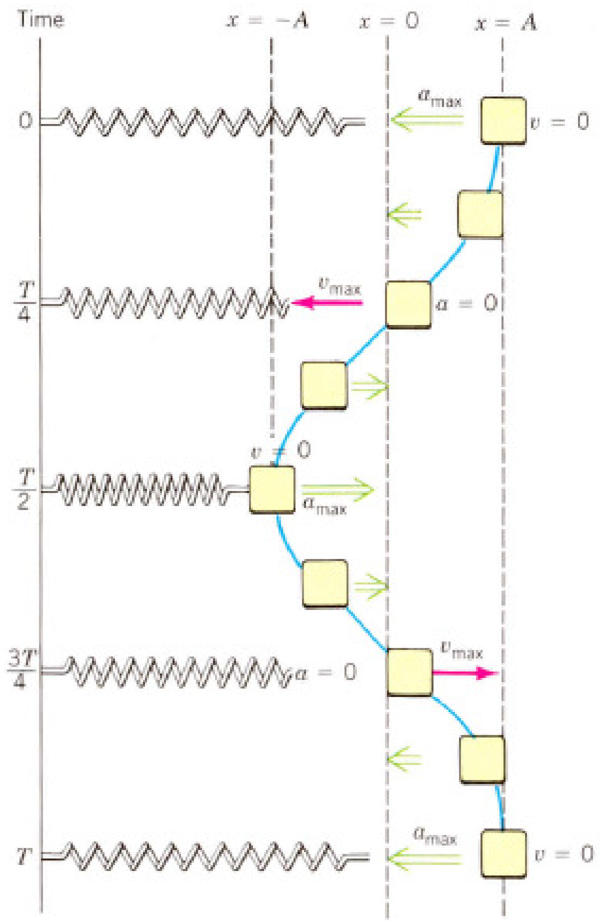
We need two constraints to determine unknown constant $A, B\,(\text{or } C, D)$

1. Initial position: $x(0) = x_0 \longrightarrow x_0 = C$
2. Initial velocity: $\frac{dx}{dt}(0) = v_0 \longrightarrow v_0 = wD$

$$x(t) = x_0\cos(wt) + \frac{v_0}{w}\sin(wt)$$
$$= A\sin(wt + \phi)$$

where $A = \sqrt{x_0^2 + \left(\frac{v_0}{w}\right)^2}$





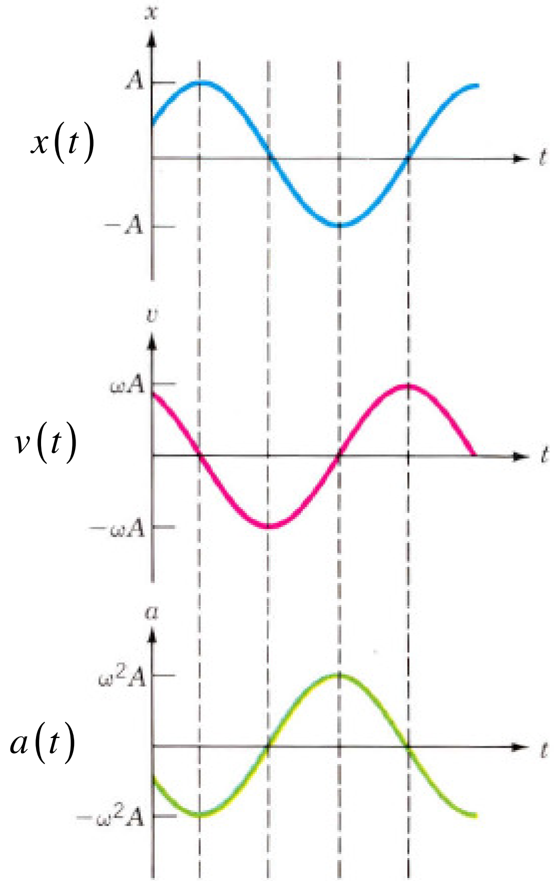
Hook's Law (虎克定律) [4]

Simple Harmonic Oscillation:

$$x(t) = A\sin(wt+\phi)$$

$$v(t) = \frac{dx}{dt} = Aw\cos(wt+\phi)$$

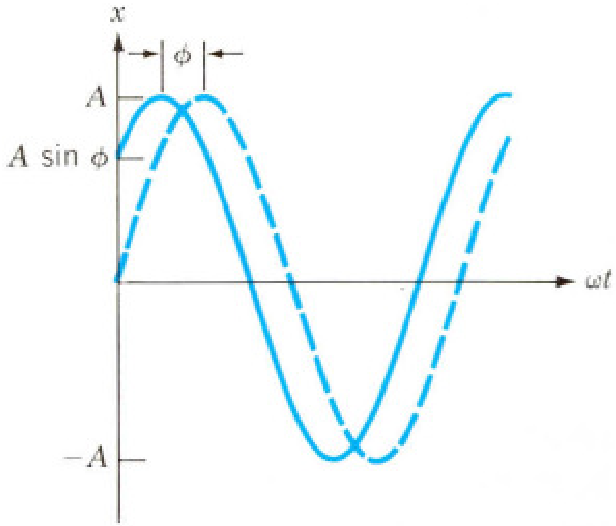
$$a(t) = \frac{d^2x}{dt^2} = -w^2x$$



$x(t)$ is shifted by phase constant ϕ

the argument $wt+\phi$ is phase (相位)

measured in radians (弧度)



Question 1: why do we guess $x = \exp(\lambda t)$ in equation $\frac{d^2x}{dt^2} + w^2x = 0$

Question 2: where do two constant A, B (or C,D) come from?

Question 3: is the solution unique?

ODE [1]

First order linear ODE: $\dfrac{dx}{dt} = \lambda x$

1 First order : highest degree of differential operation $\dfrac{dx}{dt}$ is first derivative.

2 Linear : define operator $L[x] = \dfrac{dx}{dt} - \lambda x$, then operator is linear, say $L[\alpha x] = \alpha L[x]$, $L[x+y] = L[x] + L[y]$

$$\frac{dx}{dt} = \lambda x \longrightarrow \frac{dx}{x} = \lambda dt \longrightarrow \int_{x(t_0)}^{x(T)} \frac{dx}{x} = \int_{t_0}^{T} \lambda dt$$

integration along curve $x(t)$, t_0 : initial time, T : final time

$$\longrightarrow \log\left(\frac{x(T)}{x(t_0)}\right) = \lambda(T - t_0) \longrightarrow x(T) = x(t_0)\exp[\lambda(T - t_0)]$$

Observation1: when initial time is determined and initial condition $x(t_0)$ is given, then solution $x(t)$ $\forall t$ is unique

However when initial condition is specified, then initial time is determined at once, hence we say

$x(t) = x(t_0)\exp[\lambda(t - t_0)]$ is one-parameter family, with parameter $x(t_0)$

First order linear ODE system of dimension two: $\dfrac{d}{dt}\begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} \lambda_1 & \\ & \lambda_2 \end{pmatrix}\begin{pmatrix} x_1 \\ x_2 \end{pmatrix}$

3 ODE system: more than one equation

4 system of dimension two: two equations

solution is $\begin{cases} x_1(t) = x_1(t_0)\exp[\lambda_1(t - t_0)] \\ x_2(t) = x_2(t_0)\exp[\lambda_2(t - t_0)] \end{cases}$ since system is de-couple $\begin{cases} \dfrac{dx_1}{dt} = \lambda_1 x_1 \\ \dfrac{dx_2}{dt} = \lambda_2 x_2 \end{cases}$

ODE [2]

$$\frac{d}{dt}\begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} \lambda_1 & \\ & \lambda_2 \end{pmatrix}\begin{pmatrix} x_1 \\ x_2 \end{pmatrix}$$ has unique solution if two initial conditions are specified

$$x_1(t) = x_1(t_0)\exp[\lambda_1(t-t_0)]$$
$$x_2(t) = x_2(t_0)\exp[\lambda_2(t-t_0)]$$

→

$$\begin{pmatrix} x_1 \\ x_2 \end{pmatrix}(t) = \begin{pmatrix} \exp[\lambda_1(t-t_0)] & \\ & \exp[\lambda_2(t-t_0)] \end{pmatrix}\begin{pmatrix} x_1(t_0) \\ x_2(t_0) \end{pmatrix}$$

↓

$$\exp(x) = 1 + x + \frac{x^2}{2!} + \frac{x^3}{3!} + \cdots$$ we define $\exp(A) \equiv I + A + \frac{A^2}{2!} + \frac{A^3}{3!} + \cdots$ for square matrix ***A***

let $A = \begin{pmatrix} \lambda_1 & \\ & \lambda_2 \end{pmatrix}$, then $A^n = \begin{pmatrix} \lambda_1^n & \\ & \lambda_2^n \end{pmatrix}$ implies $\exp(A(t-t_0)) = \begin{pmatrix} \exp[\lambda_1(t-t_0)] & \\ & \exp[\lambda_2(t-t_0)] \end{pmatrix}$

$$\begin{pmatrix} x_1 \\ x_2 \end{pmatrix}(t) = \exp(A(t-t_0))\begin{pmatrix} x_1(t_0) \\ x_2(t_0) \end{pmatrix}$$

Observation 2: ODE system of dimension **two** needs **two** initial conditions

Observation 3: if we write $\vec{x}(t) \equiv \begin{pmatrix} x_1 \\ x_2 \end{pmatrix}(t)$, then $\vec{x}(t) = \exp(A(t-t_0))\vec{x}(t_0)$ is unique solution of $\frac{d}{dt}\vec{x} = \begin{pmatrix} \lambda_1 & \\ & \lambda_2 \end{pmatrix}\vec{x}$, $\vec{x}(t_0)$ is given

we may guess that $\vec{x}(t) = \exp(A(t-t_0))\vec{x}(t_0)$ is unique solution of $\frac{d}{dt}\vec{x} = A\vec{x}$, $\vec{x}(t_0)$ is given, for any square matrix ***A***

ODE [3]

Simple Harmonic Oscillation: $\frac{d^2x}{dt^2} + w^2 x = 0$ where $w = \sqrt{\frac{k}{m}} \equiv 2\pi f$

Intuition: we CANNOT determine $x(t)$ by given initial position $x(0) = x_0$ since initial velocity would also affect $x(t)$

It is well-known when you are in junior high school, not only free fall experiment but sliding car experiment.

Transformation between second order ODE and first order ODE system of dimension two

Define velocity $v(t) = \frac{dx}{dt}$, then combine Newton' second Law $F = ma$, we have

$$\begin{cases} v(t) = \frac{dx}{dt} \\ \frac{d^2x}{dt^2} + w^2 x = 0 \end{cases} \longrightarrow \frac{d}{dt}\begin{pmatrix} x \\ v \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ -w^2 & 0 \end{pmatrix}\begin{pmatrix} x \\ v \end{pmatrix}$$

we need two initial condition to have unique solution

$$I.C. \begin{pmatrix} x(0) \\ v(0) \end{pmatrix}$$

From Symbolic toolbox in MATLAB, we can diagonalize matrix

$$\begin{pmatrix} 0 & 1 \\ -w^2 & 0 \end{pmatrix} = V \begin{pmatrix} iw & \\ & -iw \end{pmatrix} V^{-1}$$

where $V = \begin{pmatrix} 1 & 1 \\ iw & -iw \end{pmatrix}$, $V^{-1} = \frac{1}{-2iw}\begin{pmatrix} -iw & -1 \\ -iw & 1 \end{pmatrix}$

MATLAB code

```
syms w ;   % define w is a symbol

A = [ 0 1 ; - w^2 0 ] ;

[V,D] = eig(A) ;
```

ODE [4]

Formal deduction: $\frac{d}{dt}\begin{pmatrix} x \\ v \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ -w^2 & 0 \end{pmatrix}\begin{pmatrix} x \\ v \end{pmatrix}$ $\xrightarrow{\begin{pmatrix} 0 & 1 \\ -w^2 & 0 \end{pmatrix} = V\begin{pmatrix} iw & \\ & -iw \end{pmatrix}V^{-1}}$ $\frac{d}{dt}\left[V^{-1}\begin{pmatrix} x \\ v \end{pmatrix}\right] = \begin{pmatrix} iw & 0 \\ 0 & -iw \end{pmatrix}\cdot\left[V^{-1}\begin{pmatrix} x \\ v \end{pmatrix}\right]$

$\xrightarrow{z \equiv V^{-1}\begin{pmatrix} x \\ v \end{pmatrix} = \begin{pmatrix} z_1 \\ z_2 \end{pmatrix}}$ $\frac{d}{dt}\begin{pmatrix} z_1 \\ z_2 \end{pmatrix} = \begin{pmatrix} iw & 0 \\ 0 & -iw \end{pmatrix}\cdot\begin{pmatrix} z_1 \\ z_2 \end{pmatrix}$ with initial condition $\begin{pmatrix} z_1(0) \\ z_2(0) \end{pmatrix} = V^{-1}\begin{pmatrix} x(0) \\ v(0) \end{pmatrix}$

$\longrightarrow \begin{pmatrix} z_1 \\ z_2 \end{pmatrix} = \begin{pmatrix} \exp(iwt) & 0 \\ 0 & \exp(-iwt) \end{pmatrix}\begin{pmatrix} z_1(0) \\ z_2(0) \end{pmatrix}$ $\longrightarrow \begin{pmatrix} x \\ v \end{pmatrix} = V\begin{pmatrix} \exp(iwt) & 0 \\ 0 & \exp(-iwt) \end{pmatrix}V^{-1}\begin{pmatrix} x(0) \\ v(0) \end{pmatrix}$

Definition: fundamental matrix $\Phi \equiv V\begin{pmatrix} \exp(iwt) & 0 \\ 0 & \exp(-iwt) \end{pmatrix}V^{-1} = \exp(At) = \begin{pmatrix} \cos(wt) & \sin(wt)/w \\ -w\sin(wt) & \cos(wt) \end{pmatrix}$

then solution can be expressed by fundamental matrix and initial condition $\begin{pmatrix} x \\ v \end{pmatrix}(t) = \Phi(t)\begin{pmatrix} x(0) \\ v(0) \end{pmatrix}$

From Symbolic toolbox in MATLAB,
we can compute fundamental matrix easily

```
syms w real;   % define w is a symbol
syms t real;

A = [ 0 1 ; - w^2 0 ] ;

[V,D] = eig(A) ;

D = diag(D) ;

psi = V* diag( exp(D*t) ) * inv(V) ; % fundamental matrix

psi = simplify( psi ) ;
```

ODE [5]

fundamental matrix $\Phi = \begin{pmatrix} \cos(wt) & \sin(wt)/w \\ -w\sin(wt) & \cos(wt) \end{pmatrix} = \begin{pmatrix} \varphi & \psi \\ \frac{d}{dt}\varphi & \frac{d}{dt}\psi \end{pmatrix}$ is composed of two fundamental solutions

$\begin{pmatrix} \varphi \\ \frac{d}{dt}\varphi \end{pmatrix}$ is solution of $\frac{d}{dt}\begin{pmatrix} x \\ v \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ -w^2 & 0 \end{pmatrix}\begin{pmatrix} x \\ v \end{pmatrix}$ with initial condition $\begin{pmatrix} x(0) \\ v(0) \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$

$\begin{pmatrix} \psi \\ \frac{d}{dt}\psi \end{pmatrix}$ is solution of $\frac{d}{dt}\begin{pmatrix} x \\ v \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ -w^2 & 0 \end{pmatrix}\begin{pmatrix} x \\ v \end{pmatrix}$ with initial condition $\begin{pmatrix} x(0) \\ v(0) \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$

solution of $\frac{d}{dt}\begin{pmatrix} x \\ v \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ -w^2 & 0 \end{pmatrix}\begin{pmatrix} x \\ v \end{pmatrix}$ with initial condition $\begin{pmatrix} x(0) \\ v(0) \end{pmatrix} = \begin{pmatrix} x_0 \\ v_0 \end{pmatrix}$ is linear combination of fundamental solutions

$$x(t) = x_0\varphi(t) + v_0\psi(t) = e_1^T\Phi(t)\begin{pmatrix} x_0 \\ v_0 \end{pmatrix}$$

The space of solutions of $\frac{d}{dt}\begin{pmatrix} x \\ v \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ -w^2 & 0 \end{pmatrix}\begin{pmatrix} x \\ v \end{pmatrix}$ is $M \triangleq \left\{ \Phi(t)\begin{pmatrix} x_0 \\ v_0 \end{pmatrix} : x_0 \in R, v_0 \in R \right\} \sim R^2$

The dimension of solution space is two, $\dim M = \dim(R^2) = 2$

ODE [6]

$$\frac{d^2x}{dt^2}+w^2x=0 \longrightarrow \frac{dx}{dt}(t)=\frac{dx}{dt}(0)-\int_0^t w^2x(s)\,ds \longrightarrow x(t)=x(0)+t\cdot\frac{dx}{dt}(0)-\int_0^t\int_0^{s_2} w^2x(s_1)\,ds_1ds_2$$

In order to achieve uniqueness, we need to specify two integration constant $x(0),\frac{dx}{dt}(0)$

differential equation: $\frac{d^2x}{dt^2}+w^2x=0 \longleftrightarrow$ Integral equation: $x(t)=x(0)+t\cdot\frac{dx}{dt}(0)-\int_0^t\int_0^{s_2} w^2x(s_1)\,ds_1ds_2$

Existence and uniqueness (Contraction mapping principle)

Let $C([0,T])=\{f:[0,T]\to R \text{ is continuous}\}$ be continuous space equipped with norm $\|f\|_\infty=\max\{|f(t)|:0\le t\le T\}$

1. $C([0,T])$ is complete under norm $\|f\|_\infty=\max\{|f(t)|:0\le t\le T\}$

2. define a mapping $T:C[0,T]\to C[0,T]$ by $(Tx)(t)=x(0)+t\cdot\frac{dx}{dt}(0)-\int_0^t\int_0^{s_2} w^2x(s_1)\,ds_1ds_2$

then $(Tx-Ty)(t)=w^2\int_0^t\int_0^{s_2}\left[x(s_1)-y(s_1)\right]ds_1ds_2$

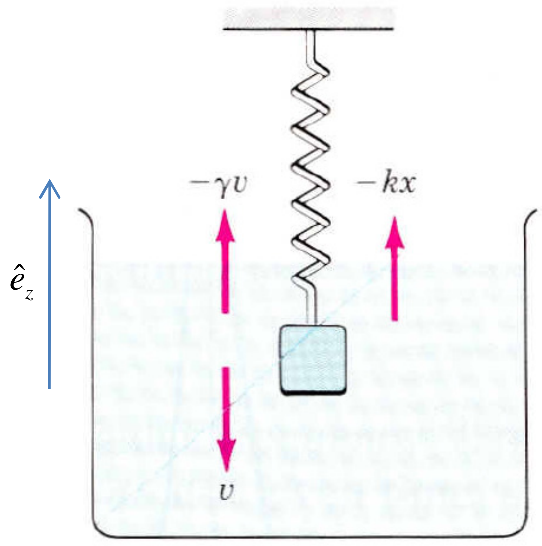
$$\downarrow$$

$$|(Tx-Ty)(t)|\le w^2\|x-y\|_\infty\int_0^t\int_0^{s_2}ds_1ds_2=\frac{t^2}{2}w^2\|x-y\|_\infty$$

$$\downarrow$$

$\|Tx-Ty\|_\infty\le\frac{T^2}{2}w^2\|x-y\|_\infty \longrightarrow T$ is a contraction mapping if $\frac{T^2}{2}w^2<1 \longrightarrow$ *Existence and uniqueness*

ODE [7]



$\vec{F} = \vec{F}_{sping} + \vec{F}_{resistence}$ (ignore buoyancy 浮力)

$\vec{F}_{sping} = -k\vec{x}$ recover force is opposite to displacement

$\vec{F}_{resistence} = -\gamma \frac{d}{dt}\vec{x}$ resistive force is also opposite to displacement

γ: damping constant

Newton second's Law: $-kx - \gamma \frac{dx}{dt} = m\frac{d^2x}{dt^2}$

1. what is equivalent ODE system of $m\frac{d^2x}{dt^2} + \gamma\frac{dx}{dt} + kx = 0$
2. what is fundamental matrix of this ODE system, use symbolic toolbox in MATALB
3. what is solution of $m\frac{d^2x}{dt^2} + \gamma\frac{dx}{dt} + kx = 0$ with initial condition $x(0) = x_0$, $\frac{dx}{dt}(0) = v_0$
4. Can you use "contraction mapping principle" to prove existence and uniqueness?

ODE [7]

$$\frac{d^2x}{dt^2} + w^2 x = 0 \longrightarrow \text{general solution} \quad x(t) = A\cos(wt) + B\sin(wt)$$

We have two choices to determine unknown constants ***A*** and ***B***

1 initial condition $\begin{pmatrix} x(0) \\ v(0) \end{pmatrix} = \begin{pmatrix} x_0 \\ v_0 \end{pmatrix} \longrightarrow x(t) = x_0 \cos(wt) + v_0 \frac{1}{w} \sin(wt)$

2 boundary condition $\begin{pmatrix} x(0) \\ x(\pi) \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$

$$x(0) = 0 \xrightarrow{x(t) = A\cos(wt) + B\sin(wt)} A = 0 \longrightarrow x = B\sin(wt)$$

$$x(\pi) = 0 \xrightarrow{x(t) = B\sin(wt)} \sin(w\pi) = 0 \longrightarrow w_n = n = 1, 2, 3\cdots \longrightarrow \text{period} \quad T_n = \frac{2\pi}{n}$$

1 Why does angular frequency $w_n = n = 1, 2, 3\cdots$ become discrete?

What is physical meaning of discrete angular frequency?

2 We have still a constant ***B*** not be determined, why?

Schrodinger equation [1]

photon (光子):
- energy $E = \hbar w$ — $w = 2\pi f$ is angular frequency
- momentum $p = \hbar k$ — $k = \dfrac{2\pi}{\lambda}$ is wave number

$h(\text{Planck's constant}) = 6.624\times 10^{-34}\, J\cdot s$

$\hbar = \dfrac{h}{2\pi}$

http://en.wikipedia.org/wiki/Matter_wave

Louis de Broglie in 1924 in his PhD thesis claims that "matter (object)" has the same relation as photon

- de Broglie wavelength $\lambda = \dfrac{p}{h}$
- de Broglie frequency of the wave $f = \dfrac{E}{h}$

Fundamental of quantum mechanic: matter wave (物質波) is described by wave length λ and wave frequency f

http://en.wikipedia.org/wiki/Schr%C3%B6dinger_equation

Erwin Schrödinger in 1926 proposed a differential equation (called Schrodinger equation) to describe atomic systems.

total energy of a particle $E = T + V = \dfrac{p^2}{2m} + V$ $\quad T: \text{kinetic energy} \quad V: \text{potential energy}$

matter wave $\psi(x,t) = A\exp(ikx - iwt)$

$$i\hbar\frac{\partial}{\partial t}\psi(x,t) = \hbar w\psi(x,t) = E\psi(x,t) \quad \text{and} \quad \frac{\hbar}{i}\frac{\partial}{\partial x}\psi(x,t) = \hbar k\psi(x,t) = p\psi(x,t)$$

$$E\psi = \left(\frac{p^2}{2m} + V\right)\psi \longrightarrow i\hbar\frac{\partial}{\partial t}\psi(x,t) = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi + V\psi$$

← time-dependent Schrodinger equation

Schrodinger equation [2]

Question: physical interpretation of matter wave $\psi(x,t)$?

$$P(x,t) \triangleq |\psi(x,t)|^2 = \text{ probability finding particle on interval } (x-\Delta x, x+\Delta x) \text{ in time } t$$

$$N(t) \equiv \int_{-\infty}^{\infty} P(x,t)\,dx = \text{total number of particles in time } t$$

Example: plane wave $\psi(x,t) = A\exp(ikx - iwt)$

$$P(x,t) \triangleq |\psi(x,t)|^2 = |A|^2 : \text{ particle has the same probability found in any position, not physical}$$

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time-dependent Schrodinger equation $i\hbar\frac{\partial}{\partial t}\psi(x,t) = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi + V\psi$

↓ remove ***t***-dependence, replace $i\hbar\frac{\partial}{\partial t}\psi(x,t)$ by $E\psi(x,t)$

time-independent Schrodinger equation $-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) + V\psi(x) = E\psi(x)$ (one-dimensional)

$$-\frac{\hbar^2}{2m}\nabla^2\psi(\vec{x}) + V\psi(\vec{x}) = E\psi(\vec{x}) \quad \text{(three-dimensional)} \quad \nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$$

Objective of time-independent Schrodinger equation: find a stationary solution satisfying

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) + V\psi(x) = E\psi(x) \quad \text{with proper boundary conditions}$$

Schrodinger equation [3]

Example: Hydrogen atom (氫原子)

$$\begin{cases} -\dfrac{\hbar^2}{2m_e}\nabla^2\psi(\vec{x})+V\psi(\vec{x})=E\psi(\vec{x}) \\ V=-\dfrac{e^2}{r}: proton-electron \\ \text{B.C.}\quad \psi(|\vec{x}|\to\infty)=0 \end{cases}$$

discrete energy level: $E_n=-\dfrac{13.6eV}{n^2}$

parameter

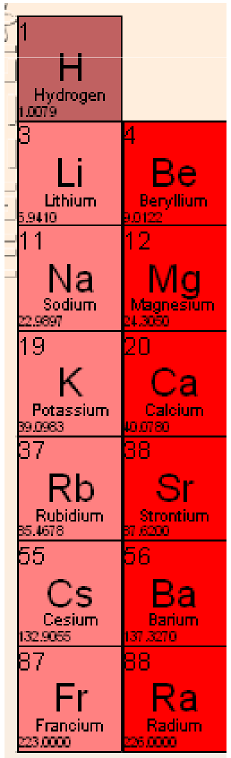
$\hbar=1.0542\times10^{-34}\,J\cdot s$

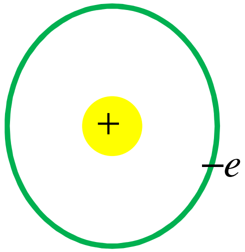
$m_e\,(\text{mass of electron})=9.1\times10^{-31}\,kg$

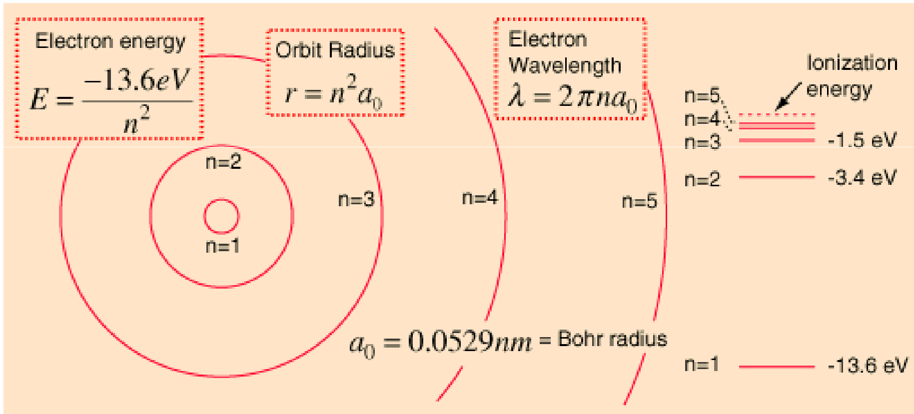
$e\,(\text{charge of electron})=1.6\times10^{-19}\,coulomb=4.8\times10^{-10}\,statecoulomb$

$1eV\,(\text{電子伏特})=1.6\times10^{-19}\,J$

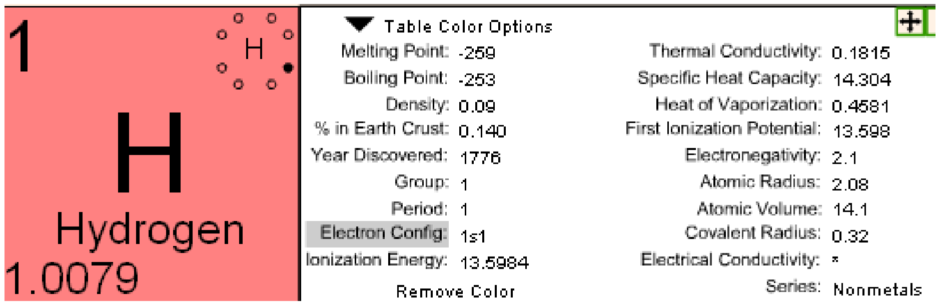
http://hyperphysics.phy-astr.gsu.edu/hbase/hyde.html







http://www.touchspin.com/chem/SWFs/pt2k61012.swf



Schrodinger equation [4]

Time-independent Schrodinger equation

$$\left(-\frac{\hbar^2}{2m_e}\Delta + V(\vec{x})\right)\psi(\vec{x}) = E\psi(\vec{x})$$

$$h = 2\pi\hbar = 6.624\times10^{-34}\,J\cdot s$$

$$m_e\,(\text{mass of electron}) = 9.1\times10^{-31}\,kg$$

$\psi(\vec{x})$: wave function, $|\psi(\vec{x})|^2$: probability of particle appears in $(\vec{x}, \vec{x}+d\vec{x})$, dimensionless quantity

From dimensional analysis, we extract dimensionless quantities in this system

1 $\vec{x} = a\vec{y}$, or say $[\vec{x}] = a$ 2 $E = \varepsilon\tilde{E}$, or say $[E] = \varepsilon$ 3 $[V] = [E]$ 4 $\psi = \text{dimensionless}$

$$\left(-\frac{\hbar^2}{2ma^2}\Delta_y + V(a\tilde{y})\right)\psi(a\tilde{y}) = \varepsilon\tilde{E}\psi(a\tilde{y})$$

↓ dimensionless form

$$\left(-\frac{1}{2}\Delta_y + \frac{ma^2}{\hbar^2}V(a\tilde{y})\right)\psi(a\tilde{y}) = \frac{ma^2\varepsilon}{\hbar^2}\tilde{E}\psi(a\tilde{y})$$

Once characteristic length of the system is determined, for example $a = 10^{-10}m = 1A^0$

Then characteristic energy is $\varepsilon = \dfrac{\hbar^2}{ma^2} \sim 10^{-18}J \sim 7eV$, this is near $E_n = -\dfrac{13.6eV}{n^2}$

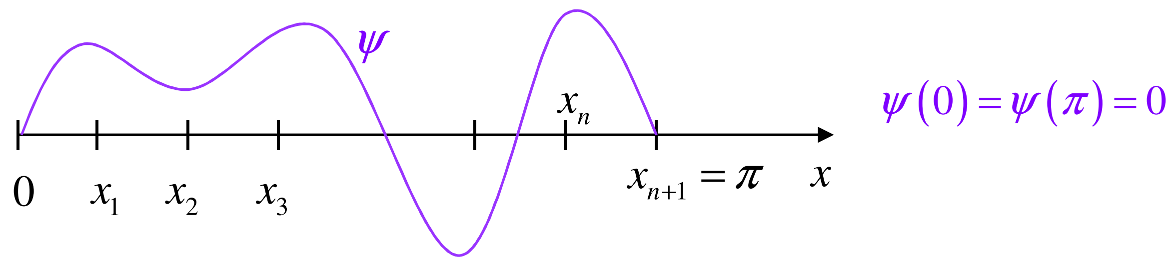
Finite Difference Method [1]

First we consider one-dimensional problem (dimensionless form)

$$\left(-\frac{1}{2}\frac{d^2}{dx^2}+V(x)\right)\psi(x)=E\psi(x),\quad \psi(0)=\psi(\pi)=0$$

Finite Difference Method (有限差分法): divide interval $[0,\pi]$ into *N+1* uniform segments

labeled as $x_0=0<x_1<x_2<\cdots<x_n<x_{n+1}=\pi,\quad x_j=jh,\ h=\frac{\pi}{n+1}$



We approximate ODE on finite points, say we want to find a vector $\left\{\psi_j=\psi(x_j):j=0,1,2,\cdots\right\}$ satisfying

$$-\frac{1}{2}\frac{d^2\psi}{dx^2}(x_j)+V(x_j)\psi(x_j)=E\psi(x_j),\quad \psi(0)=\psi(\pi)=0 \quad \text{for } j=1,2,\cdots,n$$

1. We don't need to ask equation on end points, since equation only holds in interior
2. How to approximate second derivative $\frac{d^2\psi}{dx^2}(x_j)$ on grid points
3. How to achieve "solvability" though we know solution indeed exists in continuous sense

Finite Difference Method [2]

$$f(x+h) = f + hf^{(1)} + \frac{h^2}{2} f^{(2)} + \frac{h^3}{3!} f^{(3)} + \frac{h^4}{4!} f^{(4)} + \frac{h^5}{5!} f^{(5)} + O(h^6)$$

$$+ \big) \quad f(x-h) = f - hf^{(1)} + \frac{h^2}{2} f^{(2)} - \frac{h^3}{3!} f^{(3)} + \frac{h^4}{4!} f^{(4)} - \frac{h^5}{5!} f^{(5)} + O(h^6)$$

$$f(x+h) + f(x-h) = 2\left(f(x) + \frac{h^2}{2} f^{(2)} + \frac{h^4}{4!} f^{(4)} + O(h^6) \right)$$

$$\downarrow$$

$$\frac{f(x+h) - 2f(x) + f(x-h)}{h^2} = f^{(2)}(x) + \frac{h^2}{12} f^{(4)} + O(h^4)$$

Definition: standard 3-point centered difference formula $D_h^2 f(x) \equiv \dfrac{f(x+h) - 2f(x) + f(x-h)}{h^2}$

we have $D_h^2 f(x) = f^{(2)}(x) + \dfrac{h^2}{12} f^{(4)}(c)$ for some $c \in (x-h, x+h)$

$$\uparrow$$

$\dfrac{h^2}{12} f^{(4)}(c)$ is called local truncation error (*LTE*) since it is truncation from Taylor's expansion

Finite Difference Method [3]

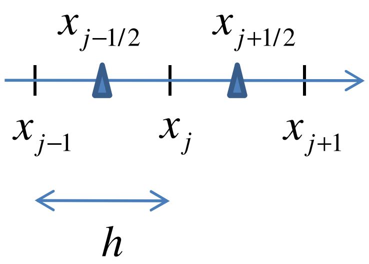
$$f(x+h) = f + hf^{(1)} + \frac{h^2}{2} f^{(2)} + \frac{h^3}{3!} f^{(3)} + \frac{h^4}{4!} f^{(4)} + \frac{h^5}{5!} f^{(5)} + O(h^6)$$

$$-\Big)\quad f(x-h) = f - hf^{(1)} + \frac{h^2}{2} f^{(2)} - \frac{h^3}{3!} f^{(3)} + \frac{h^4}{4!} f^{(4)} - \frac{h^5}{5!} f^{(5)} + O(h^6)$$

$$f(x+h) - f(x-h) = 2\left(hf^{(1)} + \frac{h^3}{3!} f^{(3)} + O(h^5) \right)$$

$$\downarrow$$

$$D_h^1 f(x) \equiv \frac{f(x+h) - f(x-h)}{2h} = f^{(1)}(x) + \frac{h^2}{6} f^{(3)} + O(h^4)$$



$$\frac{d^2 f}{dx^2}(x) = \frac{\frac{df}{dx}(x_{j+1/2}) - \frac{df}{dx}(x_{j-1/2})}{h} - \frac{h^2}{6}\left(\frac{df}{dx}\right)^{(3)} + O(h^4)$$ short-stencil

$$\frac{df}{dx}(x_{j+1/2}) = \frac{f(x_{j+1}) - f(x)}{h} - \frac{h^2}{6} f^{(3)}(x_{j+1/2}) + O(h^4)$$

$$\frac{df}{dx}(x_{j-1/2}) = \frac{f(x_j) - f(x_{j-1})}{h} - \frac{h^2}{6} f^{(3)}(x_{j-1/2}) + O(h^4)$$

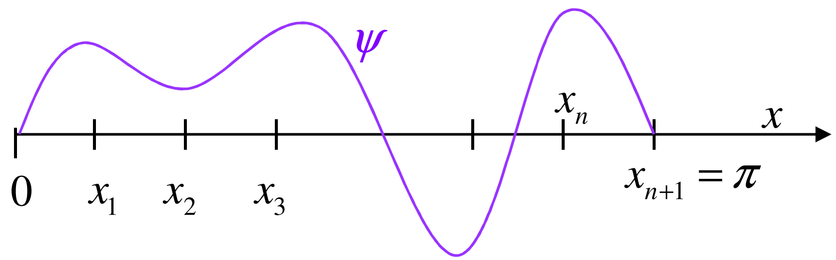
$$f^{(3)}(x_{j+1/2}) - f^{(3)}(x_{j-1/2}) = hf^{(4)}(x) + O(h^3)$$

$$\downarrow$$

$$D_h^2 f(x) = f^{(2)}(x) + \frac{h^2}{12} f^{(4)}(x) + O(h^4)$$

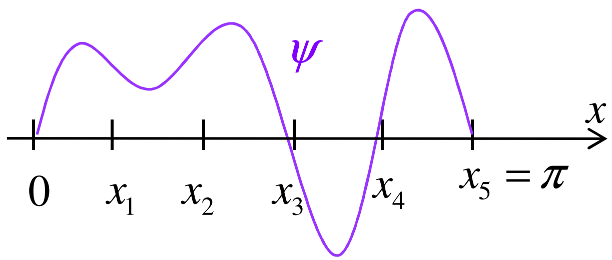
Finite Difference Method [4]

$$\begin{cases} -\dfrac{1}{2}\dfrac{d^2\psi}{dx^2}(x_j)+V(x_j)\psi(x_j)=E\psi(x_j), \quad \psi(0)=\psi(\pi)=0 \quad \text{for } j=1,2,\cdots,n \\ D_h^2\psi(x)=\psi^{(2)}(x)+\dfrac{h^2}{12}\psi^{(4)}(c) \end{cases}$$



$$\rightarrow \left\{-\frac{1}{2h^2}\begin{pmatrix} -2 & 1 & & \\ 1 & -2 & 1 & \\ & & \ddots & \\ & & 1 & -2 \end{pmatrix}+diag(V)\right\}\vec{\psi}=E\vec{\psi}$$

Example: n = 4



$$\underbrace{\left\{-\frac{1}{2h^2}\begin{pmatrix} -2 & 1 & & \\ 1 & -2 & 1 & \\ & 1 & -2 & 1 \\ & & 1 & -2 \end{pmatrix}+\begin{pmatrix} V_1 & & & \\ & V_2 & & \\ & & V_3 & \\ & & & V_4 \end{pmatrix}\right\}}_{A}\begin{pmatrix}\psi_1\\ \psi_2\\ \psi_3\\ \psi_4\end{pmatrix}=E\begin{pmatrix}\psi_1\\ \psi_2\\ \psi_3\\ \psi_4\end{pmatrix}$$

$A\vec{\psi}=E\vec{\psi}$ $\quad$ A is real symmetric, then ***A*** is diagonalizable since eigenvalue of A is real

Finite Difference Method [5]

model problem: no potential (V = 0)

$$-\frac{1}{2}\frac{d^2\psi}{dx^2}(x)=E\psi(x),\quad \psi(0)=\psi(\pi)=0 \quad \xrightarrow{\text{FDM}} \quad -\frac{1}{2h^2}\begin{pmatrix} -2 & 1 & & \\ 1 & -2 & 1 & \\ & & \ddots & \\ & & 1 & -2 \end{pmatrix}\bar{\psi}=E\bar{\psi}$$

Question: can we find analytic formula for eigen-pair in this simple model problem?

$$\frac{d^2x}{dt^2}+w^2x=0,\quad x(0)=x(\pi)=0 \quad \longleftrightarrow \quad -\frac{d^2\psi}{dx^2}(x)=k^2\psi(x),\quad \psi(0)=\psi(\pi)=0$$

solution is $x_n(t)=\sin(w_n t) \quad w_n=n=1,2,3\cdots$

solution is $\psi_k(x)=\sin(kx) \quad k=1,2,3\cdots$

FDM ↓

$$-D_h^2\psi(x_j)=\lambda\psi(x_j) \quad \text{for} \quad j=1,2,\cdots,n \quad h=\frac{\pi}{n+1}$$

Conjecture: we guess that eigenvector is $\bar{\psi}_k=\{\sin(kx_j): j=0,1,2,\cdots,n,n+1,k\in\mathbb{N}\}$

$$D_h^2\psi_k(x_j)=\mathrm{Im}\frac{\exp(ikx_{j+1})-2\exp(ikx_j)+\exp(ikx_{j-1})}{h^2}=\mathrm{Im}\left\{\exp(ikx)\frac{\exp(ikh)-2+\exp(ikh)}{h^2}\right\}$$

$$=\frac{2\cos(kh)-1}{h^2}\mathrm{Im}\exp(ikx)=-\frac{4\sin^2(kh/2)}{h^2}\psi_k(x_j) \quad \longrightarrow \quad \lambda_k=\frac{4\sin^2(kh/2)}{h^2}$$

$\psi_k(j)=\sin(kx_j)=\sin\left(\frac{k\pi}{n+1}j\right)$ satisfies $\psi_0=\psi_{n+1}=0$ (boundary condition)

Question: How about $\bar{\psi}_k=\{\sin(kx_j): j=0,1,2,\cdots,n,n+1\}$ for $k=n+1,n+2,\cdots$

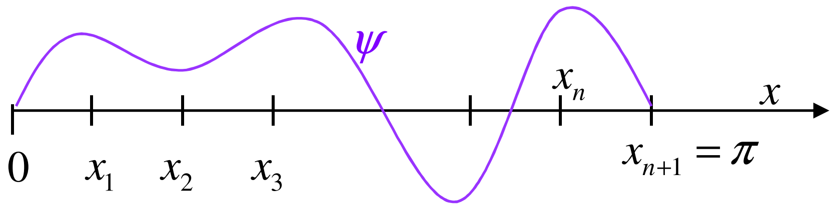
Finite Difference Method [6]

model problem: no potential (V = 0)

$$-\frac{1}{2}\frac{d^2\psi}{dx^2}(x) = E\psi(x), \quad \psi(0)=\psi(\pi)=0 \quad \xrightarrow{k=\sqrt{2E}} \quad \text{eigen-function: } \psi_k(x)=\sin(kx),\ k=1,2,3\cdots$$

Finite Difference Method on model problem:

$$-D_h^2\psi(x_j) = \lambda\psi(x_j) \quad \text{for} \quad j=1,2,\cdots,n \qquad h=\frac{\pi}{n+1}$$



eigen-pair:

$$\vec{\psi} = \{\sin(kx_j) : j=0,1,2,\cdots,n,n+1, k\in\mathbb{N}\}$$

$$\lambda_k = \frac{4\sin^2(kh/2)}{h^2} \equiv k_{num}^2$$

Question: How accurate are numerical eigen-value?

Exact wave number: $k=1,2,3\cdots,n,n+1,\cdots$

Numerical wave number: $k_{num} = \dfrac{\sin(kh/2)}{h/2}$

Taylor expansion: $\sin x = x - \dfrac{\cos(c)}{3!}x^3$ where c between 0 and x

$$k_{num} = k\frac{\sin(x)}{x}\Big|_{x=kh/2} = k - \frac{\cos(c_k)}{24}k^3h^2$$

$$\Delta k = |k-k_{num}| = \frac{|\cos(c_k)|}{24}k^3h^2 = O(k^3h^2)$$

Question: eigenvalue is second order accuracy, $\Delta k \propto h^2$, is this reasonable, why?

Question: why does error of eigenvalue increase as wave number *k* increases? $\Delta k \propto k^3$

Finite Difference Method [7]

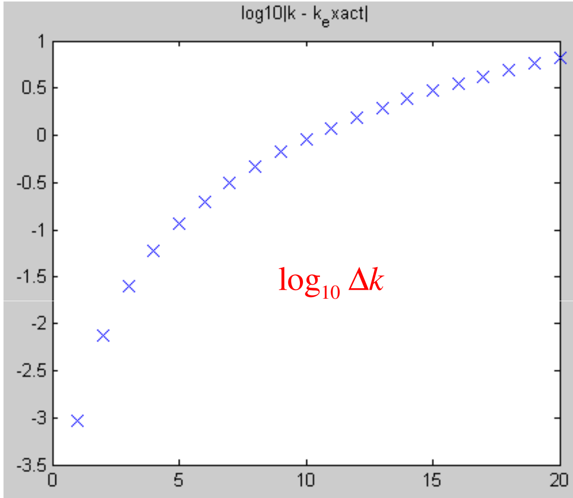
```
%
%   model problem
%      1    d^2
%  - --- ------ \psi = E \psi
%      2    dx^2


n = 20 ;
h = pi/(n+1) ; % index 0, 1, ..., n, n+1
x = 0:h:pi ;

D2 = diag( ones(n-1,1), -1 ) ;
D2 = D2 + diag( -2*ones(n,1) ) ;
D2 = D2 + diag( ones(n-1,1), 1 ) ;
D2 = -D2/h^2 ; %

T = D2/2 ;
V = diag( zeros(n,1) ) ;
A = T + V ;

[V,D] = eig(A) ;
E = diag(D) ;
k = sqrt(2*E) ;

k_exact = 1:n ;
k_exact = k_exact' ;
dk = abs( k - k_exact ) ;

alpha = dk./( k_exact.^3.*h.^2/24 ) ;

figure(1)
  plot( 1:n, log(dk)/log(10), 'x', 'MarkerSize', 10 ) ;
  title('|k - k_exact|')

figure(2)
  plot( 1:n, alpha, 'x', 'MarkerSize', 10 ) ;
  title('Big-O factor')
```

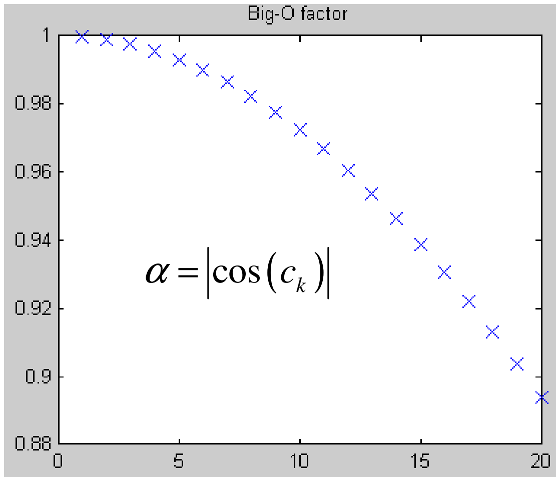
```
>> help diag
 DIAG Diagonal matrices and diagonals of a matrix.
    DIAG(V,K) when V is a vector with N components is a square matrix
    of order N+ABS(K) with the elements of V on the K-th diagonal. K = 0
    is the main diagonal, K > 0 is above the main diagonal and K < 0
    is below the main diagonal.
```

$$D_2 := \begin{pmatrix} -2 & 1 & & \\ 1 & -2 & 1 & \\ & & \ddots & \\ & & 1 & -2 \end{pmatrix}$$

model problem: no potential (V = 0)

$$\Delta k = \frac{\alpha}{24} k^3 h^2, \quad \alpha = \left|\cos(c_k)\right|$$





Exercise 1: model problem (high order accuracy)

Finite Difference Method on model problem:

$$-D_h^2\psi(x_j) = \lambda\psi(x_j) \quad \text{for} \quad j = 1, 2, \cdots, n \quad h = \frac{\pi}{n+1}$$

eigen-pair:

$$\begin{cases} \vec{\psi} = \left\{\sin(kx_j) : j = 0, 1, 2, \cdots, n, n+1, k \in \mathbb{N}\right\} \\ \lambda_k = \dfrac{4\sin^2(kh/2)}{h^2} \equiv k_{num}^2 \end{cases}$$

$$\longrightarrow \quad \Delta k = \left|k - k_{num}\right| = \frac{\left|\cos(c_k)\right|}{24} k^3 h^2 = O\left(k^3 h^2\right)$$

Question: how can we improve accuracy of eigenvalue of model problem?

Step 1: deduce 4-order centered finite difference scheme for second order derivative

$$f(x \pm h) = f \pm h f^{(1)} + \frac{h^2}{2} f^{(2)} \pm \frac{h^3}{3!} f^{(3)} + \frac{h^4}{4!} f^{(4)} \pm \frac{h^5}{5!} f^{(5)} + O\left(h^6\right)$$

$$f(x \pm 2h) = f \pm (2h) f^{(1)} + \frac{(2h)^2}{2} f^{(2)} \pm \frac{(2h)^3}{3!} f^{(3)} + \frac{(2h)^4}{4!} f^{(4)} \pm \frac{(2h)^5}{5!} f^{(5)} + O\left(h^6\right)$$

$$\downarrow$$

$$f^{(2)}(x) = \tilde{D}_h^2 f + O\left(h^4\right)$$

Step 2: can you transform continuous equation to discrete equation?

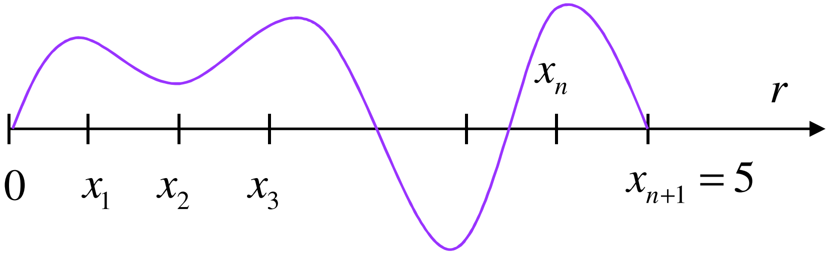
$$-\frac{1}{2}\frac{d^2\psi}{dx^2} = E\psi, \ \psi(0) = \psi(\pi) = 0 \quad \longrightarrow \quad -\tilde{D}_h^2\psi(x_j) = \lambda\psi(x_j) \quad \text{for} \quad j = 1, 2, \cdots, n \quad h = \frac{\pi}{n+1}$$

Exercise 2: singular potential

effective potential: $V_{eff}(r) = \frac{1}{r} - 140e^{-r^2}$

$$\left(-\frac{1}{2}\frac{d^2}{dr^2} + V_{eff}(r)\right)\psi(r) = E\psi(r), \quad \psi(0) = \psi(5) = 0$$

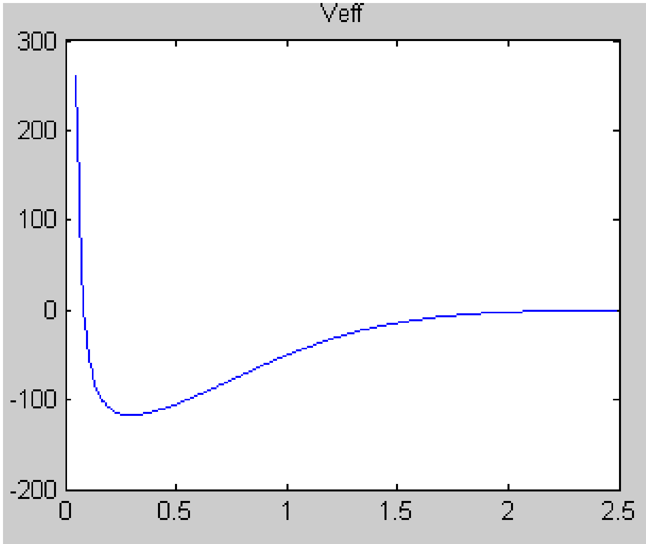
finite difference with uniform mesh $n = 1000$
platform: MATLAB



$$\left\{-\frac{1}{2h^2}\begin{pmatrix} -2 & 1 & & \\ 1 & -2 & 1 & \\ & & \ddots & \\ & & 1 & -2 \end{pmatrix} + diag\left(V_{eff}\right)\right\}\psi_l = E\psi_l$$

There are only six bound state (energy $E < 0$)

Definition: bound state means $\psi_{bound}(r \to \infty) = 0$



$E =$

E	
-100.4089	bound state
-72.4950	bound state
-48.0966	bound state
-27.5985	bound state
-11.6245	bound state
-1.4779	bound state
0.6397	
2.0966	
4.2394	
7.0023	

Exercise: plot first 10 eigen-function and interpret why only first lowest six eigenvalue corresponds to "bound state"