Schrodinger Wave Equation for the complex wave function $\Psi(x,t)$.

$$i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} + V(x)\Psi$$

This equation has separable stationary solutions.

$$\Psi(x,t) = \psi(x)\cdot\phi(t)$$

The time evolution $\phi(t)$ is simply a Phase factor： $e^{-i\frac{E}{\hbar}t}$ 。

The x-dependent $\psi(x)$ satisfies Time-Independent Schrodinger Equation：

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

對照表

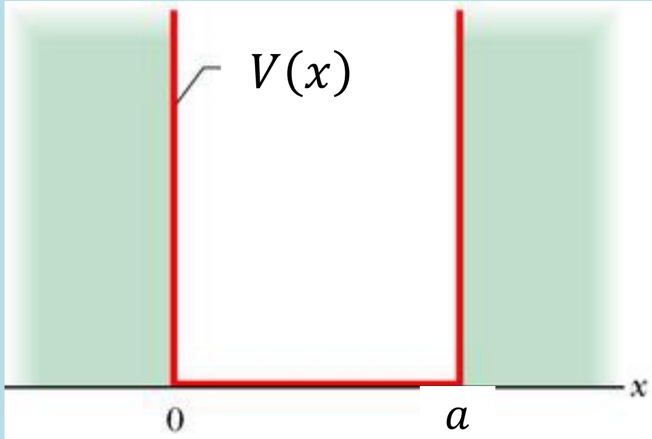
$\frac{d^2\boldsymbol{X}}{dt^2} = -\boldsymbol{A}\cdot\boldsymbol{X}$	$\frac{\partial^2\phi}{\partial t^2} = v^2\frac{\partial^2\phi}{\partial x^2}$	$i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} + V(x)\Psi$
$\boldsymbol{A}$	$\frac{d^2}{dx^2}$ 微分運算稱為算子	$\hat{H} \equiv -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)$

Time Part

$\boldsymbol{X} = \mathrm{Re}\,\boldsymbol{a}e^{i\omega t} = \boldsymbol{a}a_m\cos(\omega t + \phi)$	$\phi = X(x)\cdot\cos(\omega t + \phi)$	$\Psi = \psi(x)\cdot e^{-i\frac{E}{\hbar}t}$

Space Part

$\boldsymbol{a}$	$X(x)$	$\psi(x)$
$-\boldsymbol{A}\cdot\boldsymbol{a} = \lambda\boldsymbol{a}$	$\frac{d^2X}{dx^2} = \lambda X$	$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V\psi = E\psi$
矩陣$\boldsymbol{A}$的本徵值方程式！	算子 $\frac{d^2}{dx^2}$ 的本徵值方程式！	算子$\hat{H}$的本徵值方程式！



有邊界之自由電子

在邊界內，如同自由電子：$V(x)=0$。

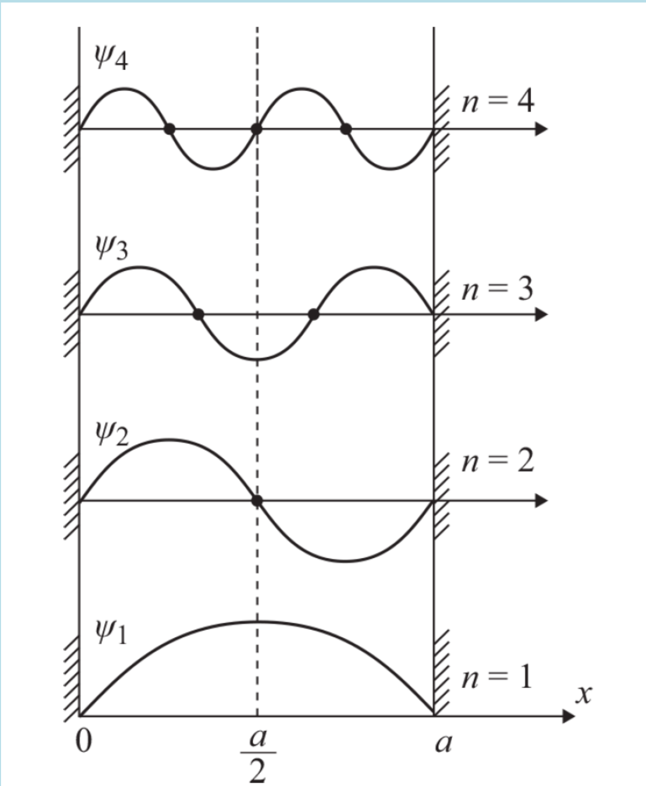
$$\frac{d^2\psi}{dx^2}=-\frac{2mE}{\hbar^2}\psi$$

若$E>0$

$$k\equiv\sqrt{\frac{2mE}{\hbar^2}}$$

$$\frac{d^2\psi}{dx^2}=-k^2\psi$$

$$\psi=Ae^{ikx}+Be^{-ikx}=C\cos kx+D\sin kx$$



邊界條件：

$$\psi(0)=0 \qquad \psi(a)=0$$

$$u_n=\sqrt{\frac{2}{a}}\sin\left(\frac{n\pi}{a}x\right)$$

只有在$k=\frac{n\pi}{a}$才有解。

$$E_n=\left(\frac{\hbar^2}{2m}\right)\frac{\pi^2}{a^2}n^2=\left(\frac{h^2}{8ma^2}\right)n^2$$

Linear combinations of stationay state are still solutions.

$$\sum_{n=1}^{\infty}a_nu_n(x)e^{-i\frac{E_n}{\hbar}t}$$

根據傅立葉分析，滿足邊界條件的任何函數$\psi(x)$，

都可以分解為正弦函數、也就是u_n的疊加！

Any function can be expanded as linear combinations of u_n, the Sine function.

This is the so-called Fourier Series. u_n, the Sine Functions are complete.

u_n具有完備性！展開定理Expansion Theorem

$$\psi(x) = \sum_{n=1}^{\infty} a_n \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a} x\right) = \sum_{n=1}^{\infty} a_n u_n(x)$$

很容易證明正弦函數u_n滿足正交定理，

$$\int_0^a dx \cdot u_n^*(x) u_m(x) = \delta_{mn}$$

分量components a_n可以利用u_n彼此正交的特性計算出來：

$$a_n = \int_0^a dx \cdot u_n^*(x)\psi(x) = \int_0^a dx \cdot \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a} x\right) \psi(x)$$

這一展開式提供對無限大位能井位能下薛丁格波方程式的普遍解法：

將$t = 0$時的波函數，即起始條件，對定態解u_n展開如下：

$$\Psi(x,0) = \sum_{n=1}^{\infty} a_n u_n(x)$$

根據展開定理，這永遠可以做到！

$t = 0$時此狀態可以視為定態u_n的如上疊加，

接著定態隨時間個自演化，位能下薛丁格方程式要求u_n乘上$e^{-i\frac{E_n}{\hbar}t}$。

乘完之後依同樣方式疊加，整個波函數也就滿足薛丁格波方程式。

$$\Psi(x,t) = \sum_{n=1}^{\infty} a_n u_n(x) e^{-i\frac{E_n}{\hbar}t}$$

=

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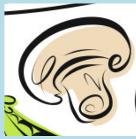


+

⋮

各個配料分離烹煮

→

若確認任一合邊界條件的函數可以本徵函數分解，我們就能計算其分解係數a_n。

但這樣的分解真的是正確的嗎？分解所得的無限級數真的與被分解的函數相等嗎？

數學上相等與否的判準：這些係數組成的u_n的線性組合，會趨近被分解的函數。

$$\lim_{N\to\infty}\int_0^L dx\left[\psi(x)-\sum_{n=1}^{N}a_n u_n(x)\right]^2=0$$

兩者差距的平方和(積分)$N\to\infty$時，趨近於零。

這稱為Completeness.完備性，必須嚴格證明的。下學期將說明。

We will extend our results in the infinite quantum well in two directions:

First, you can solve more general partial differential equation in identical way:

The fact that u_n's are orthogonal and complete is true for more general PDE.

Sturm-Liouville Problem

$$\frac{\partial}{\partial x}\left[\tau(x)\frac{\partial y}{\partial x}\right] - v(x)y = \mu(x)\frac{\partial^2 y}{\partial t^2}$$

Second, let the boundary go to infinity $a \to \infty$.

We will find a similar formalism for the space without boundary!

習題九

1. We consider String Wave Equation last term: $\tau \frac{\partial^2 y}{\partial x^2} = \mu \frac{\partial^2 y}{\partial t^2}$. It can be generalized to the case with x-dependent $\tau(x), \mu(x)$ and an extra restoring force $v(x)$. The equation is now written as:

$$\frac{\partial}{\partial x}\left[\tau(x)\frac{\partial y}{\partial x}\right] - v(x)y = \mu(x)\frac{\partial^2 y}{\partial t^2}$$

also known as generalized string wave equation.

It can be solved in ways quite similar to wave equation by separation of variables.

Assume the separable mode solutions can be written as

$$y(x,t) = X(x) \cdot T(t).$$

A. Find the Ordinary Differential Equation satisfied by $X(x)$ and $T(t)$. Show that $T(t)$ satisfies the same equation of motion as SHM and solution can be written as

$$T(t) = a_m \cos(\omega t + \phi)$$

Tension $\tau(x)$ and Mass density $\mu(x)$ could be x dependent

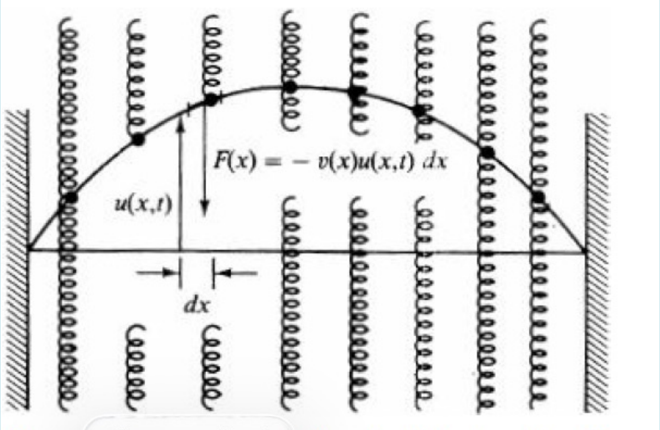
There could be extra external spring force $\propto y$ with x dependent $k = v(x)$.

Sturm-Liouville Problem

$$\frac{\partial}{\partial x}\left[\tau(x)\frac{\partial y}{\partial x}\right] - v(x)y = \mu(x)\frac{\partial^2 y}{\partial t^2} \quad \Longleftrightarrow \quad \tau\frac{\partial^2 y}{\partial x^2} = \mu\frac{\partial^2 y}{\partial t^2}$$

Tension $\tau(x)$ and Mass density $\mu(x)$ could be x dependent

There could be extra external spring force $\propto y$ with x dependent $k = v(x)$.



$$\frac{\partial}{\partial x}\left[p(x)\frac{\partial y}{\partial x}\right] - q(x)y = \mu\frac{\partial^2 y}{\partial t^2}$$

or

$$\frac{\partial}{\partial x}\left[p(x)\frac{\partial y}{\partial x}\right] - q(x)y = -i\mu\frac{\partial y}{\partial t}$$

Assume the separable mode solutions can be written as

$$y(x,t) = f(x)\cdot T(t)$$

Time part can be solved right away:

$$T(t) = a_m\cos\left(\sqrt{\lambda}t + \phi\right)$$

or

$$T(t) = e^{i\frac{\lambda}{\mu}t}$$

Space part satisfies the following equation:

術語稱為 Sturm-Liouville Problem 算子的本徵函數問題

$$\frac{d}{dx}\left[p(x)\frac{d}{dx}f(x)\right]+q(x)\cdot f(x)=\lambda\cdot f(x)$$

λ是數：本徵值，若加邊界條件下通常只有某些值，此式才有解。

$f(x)$ share the same ODE with Time-Independent Schrodinger Equation.

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2}+V(x)\psi=E\psi \qquad p(x)=-\frac{\hbar^2}{2m},\, q(x)=V(x)$$

and the space part of classical wave equation:

$$\frac{d^2X}{dx^2}=\lambda X \qquad p(x)=1,\, q(x)=0$$

Jacques Sturm 1803-1855

Joseph Liouville 1809-1882

École Polytechnique

術語稱為 Sturm-Liouville Problem 算子的本徵函數問題

$$\frac{d}{dx}\left[p(x)\frac{d}{dx}f(x)\right]+q(x)\cdot f(x)=\lambda\cdot f(x)$$

We can denote the operation on the function $f(x)$ as an operator $\hat{A}$.

$$\hat{A}\equiv\frac{d}{dx}\left[p(x)\frac{d}{dx}\right]+q(x)$$

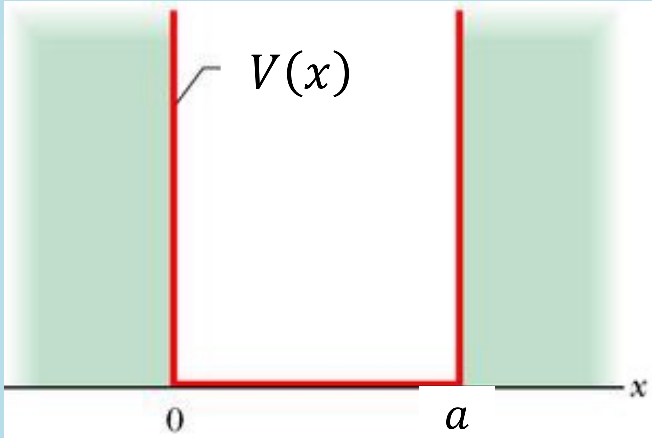
The equation can be written as:

$$\hat{A}\cdot f(x)=\lambda\cdot f(x) \quad \Longleftrightarrow \quad -\boldsymbol{A}\cdot\boldsymbol{a}=\lambda\boldsymbol{a}$$

This will be called Sturm-Liouville Eigenfunction Equation of Operator $\hat{A}$.

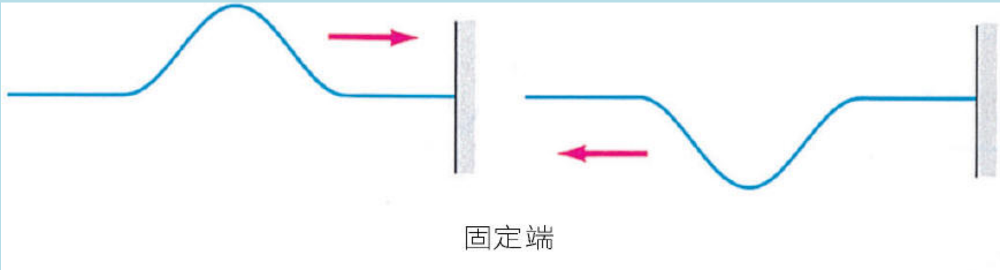
Boundary Conditions

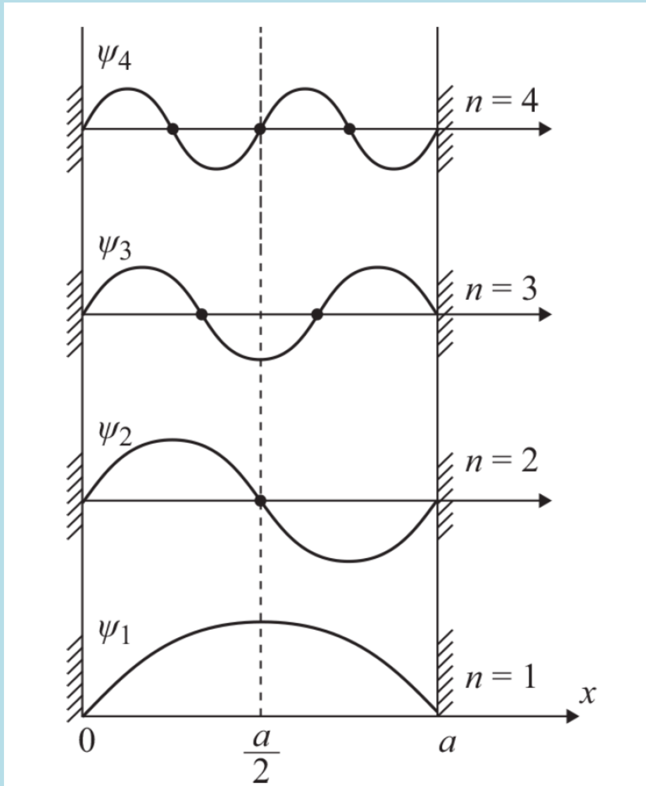
Johann Dirichlet 1805-1889



Dirichlet Condition

$$f(a) = f(b) = 0$$



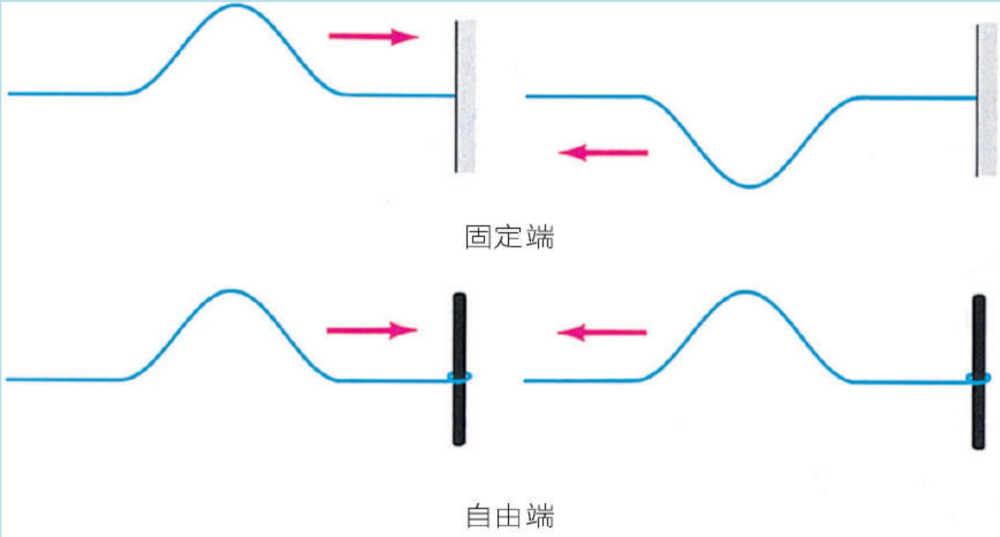


Boundary Conditions

Johann Dirichlet 1805-1889

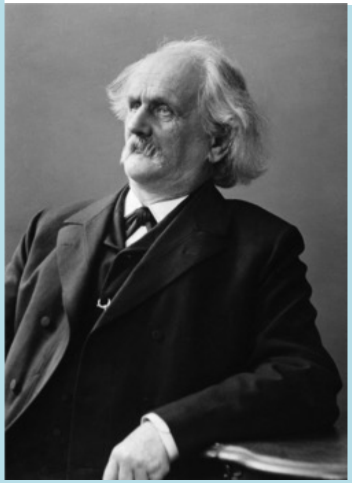
Dirichlet Condition

$$f(a) = f(b) = 0$$



Neumann Condition

$$f'(a) = f'(b) = 0$$



Carl Neumann 1832-1925

$$\hat{A} \cdot f(x) = \frac{d}{dx}\left[p(x)\frac{d}{dx}f(x)\right] + q(x)f(x) = \lambda f(x)$$

Under boundary conditions, the equation has a countable set of solutions.

We can usually classify them by natural numbers: n.

The eigenfunctions are u_n and their corresponding eigenvalues are λ_n.

$$\hat{A} \cdot u_n(x) = \lambda_n \cdot u_n(x)$$

本徵值皆為實數 Eignevalues are all real：

$$\lambda_n^* = \lambda_n$$

Time part will be oscillating: $T(t) = e^{i\frac{\lambda_n}{\mu}t}$

不同本徵值的本徵函數滿足如下正交關係，因此可取為orthonomal：

Eigenfunctions of different Eignevalues are orthogonal to each other.

$$\int_a^b dx \cdot u_n(x)^* \cdot u_m(x) = \delta_{nm}$$

Any function can be expanded as linear combinations of u_n.

u_n, the eigenfunctions are complete.

u_n具有完備性！展開定理Expansion Theorem

$$\psi(x) = \sum_{n=1}^{\infty} c_n u_n(x)$$

很容易證明正弦函數u_n滿足正交定理，

$$\int_0^a dx \cdot u_n^*(x) u_m(x) = \delta_{mn}$$

分量components c_n可以利用u_n彼此正交的特性計算出來：

$$c_n = \int_0^a dx \cdot u_n^*(x) \psi(x)$$

$$\psi(x) = \sum_{n=1}^{\infty} c_n u_n(x)$$

代入ψ的展開。

分量components c_n可以利用u_n彼此正交的特性計算出來：

$$\int_{-\infty}^{\infty} dx \cdot u_n^*(x)\psi(x) = \int_{-\infty}^{\infty} dx \cdot u_n^*(x)\left[\sum_{m=1}^{\infty} c_m u_m(x)\right]$$

$$= \sum_{m=1}^{\infty} c_m \int_{-\infty}^{\infty} dx \cdot u_n^*(x) u_m(x) = \sum_{m=1}^{\infty} c_m \delta_{mn} = c_n$$

$$c_n = \int_{-\infty}^{\infty} dx \cdot u_n^*(x)\psi(x)$$

分量c_a可以寫成態函數與本徵函數的空間積分。很像向量與基底的內積投影：

$$\hat{A} \cdot f(x) = \frac{d}{dx}\left[p(x)\frac{d}{dx}f(x)\right] + q(x)f(x) = \lambda f(x)$$

The eigenfunctions are u_n and their corresponding eigenvalues are λ_n.

$$\hat{A} \cdot u_n(x) = \lambda_n \cdot u_n(x)$$

本徵值皆為實數 Eignevalues are all real：

$$\lambda_n^* = \lambda_n$$

$\hat{A}$ 的所有本徵值λ_n都是實數！

All n eigenvalues λ of a symmetric matrix $\boldsymbol{S}$ are real.

Proof:

$$\boldsymbol{S}\boldsymbol{u} = \lambda\boldsymbol{u}$$

Take a inner product of the both sides with the complex conjugate of eigenvector $\boldsymbol{u}^*$.

$$\boldsymbol{u}^{*\mathrm{T}}\boldsymbol{S}\boldsymbol{u} = \lambda\boldsymbol{u}^{*\mathrm{T}}\boldsymbol{u}$$

$\boldsymbol{u}^{*\mathrm{T}}\boldsymbol{u} = u_1^* u_1 + u_2^* u_2$ is real. 這是複數行向量的內積，定義必定為實數。

要確認$\boldsymbol{u}^{*\mathrm{T}}\boldsymbol{S}\boldsymbol{u}$是否是實數，取他的Complex conjugate

$$\left(\boldsymbol{u}^{*\mathrm{T}}\boldsymbol{S}\boldsymbol{u}\right)^* = \left(\sum_{i,j=1}^{2} u_i^* S_{ij} u_j\right)^* = \sum_{i,j=1}^{2} u_i S_{ij}^* u_j^* = \underbrace{\sum_{i,j=1}^{2} u_j^* S_{ij} u_i}_{\boldsymbol{S}\text{實數}} = \underbrace{\sum_{i,j=1}^{2} u_j^* S_{ji} u_i}_{\text{對稱}} = \boldsymbol{u}^{*\mathrm{T}}\boldsymbol{S}\boldsymbol{u}$$

確認$\boldsymbol{u}^{*\mathrm{T}}\boldsymbol{S}\boldsymbol{u}$是實數，因此$\lambda$一定是實數。

$$\int_a^b dx \cdot u_n(x)^* \cdot \hat{A}u_n(x) = \lambda_n \int_a^b dx \cdot u_n(x)^* \cdot u_n(x)$$

$$= \int_a^b dx \cdot \left\{u_n^* \frac{d}{dx}\left[p(x)\frac{d}{dx}\right]u_n + q(x)u_n^* u_m\right\}$$

Take the complex conjugate of the above equation:

$$= \int_a^b dx \cdot \left\{u_n \frac{d}{dx}\left[p(x)\frac{d}{dx}\right]u_n^* + q(x)u_n u_n^*\right\} = \boxed{\lambda_n^* \int_a^b dx \cdot u_n^* u_n}$$

$$= \int_a^b dx \cdot \left\{-\frac{du_n}{dx} p \frac{du_n^*}{dx} + q u_n^* u_n\right\} + \left(u_n\left[p\frac{du_n^*}{dx}\right]\right)\Bigg|_a^b$$

$$= \int_a^b dx \cdot \left\{\frac{d}{dx}\left[p\frac{du_n}{dx}\right]u_n^* + q u_n u_n^*\right\} + \left(u_n^*\left[p\frac{du_n}{dx}\right]\right)\Bigg|_a^b$$

$$= \int_a^b dx \cdot \left\{\frac{d}{dx}\left[p\frac{du_n}{dx}\right] + q u_n\right\}u_n^* = \int_a^b dx \cdot [\hat{A}u_n]u_n^* \boxed{= \lambda_n \int_a^b dx \cdot u_n u_n^*}$$

$$\lambda_n^* = \lambda_n$$

$$\hat{A} \cdot f(x) = \frac{d}{dx}\left[p(x)\frac{d}{dx}f(x)\right] + q(x)f(x) = \lambda f(x)$$

The eigenfunctions are u_n and their corresponding eigenvalues are λ_n.

$$\hat{A} \cdot u_n(x) = \lambda_n \cdot u_n(x)$$

不同本徵值的本徵函數滿足如下正交關係，因此可取為orthonomal：

Eigenfunctions of different Eignevalues are orthogonal to each other.

$$\int_a^b dx \cdot u_n(x)^* \cdot u_m(x) = \delta_{nm}$$

$\hat{A}$的所有本徵函數$u_n(x)$彼此正交：

$$\int_a^b dx \cdot u_n(x)^* \cdot u_m(x) = \delta_{nm}$$

The n eigenvectors $\boldsymbol{u}$ can be chosen to be orthogonal.

Proof:

Consider two eigenvectors with different eigenvalues:

$$\boldsymbol{S}\boldsymbol{u}^{(1)} = \lambda_1 \boldsymbol{u}^{(1)} \qquad \boldsymbol{S}\boldsymbol{u}^{(2)} = \lambda_2 \boldsymbol{u}^{(2)}$$

將第一式與$\boldsymbol{u}^{(2)}$作內積，可得：

$\boldsymbol{u}^{(2)T}\boldsymbol{S}\boldsymbol{u}^{(1)} = \lambda_1 \boldsymbol{u}^{(2)T}\boldsymbol{u}^{(1)}$ $\boldsymbol{S}$作用於右邊的$\boldsymbol{u}^{(1)}$，等於本徵值λ_1相乘。

左邊可以寫成: $S_{ij} = S_{ji}$ **也等於**$\boldsymbol{S}$作用於左邊的$\boldsymbol{u}^{(2)}$，等於本徵值λ_2相乘。

$$\boldsymbol{u}^{(2)T}\boldsymbol{S}\boldsymbol{u}^{(1)} = \sum_{i,j=1}^{2} u_{2i}S_{ij}u_{1j} = \sum_{i,j=1}^{2} u_{1j}S_{ji}u_{2i} = \boldsymbol{u}^{(1)T}\cdot\boldsymbol{S}\boldsymbol{u}^{(2)} = \boldsymbol{u}^{(1)T}\lambda_2\boldsymbol{u}^{(2)} = \lambda_2\boldsymbol{u}^{(2)T}\boldsymbol{u}^{(1)}$$

得：

$$\lambda_1 \boldsymbol{u}^{(2)T}\boldsymbol{u}^{(1)} = \lambda_2 \boldsymbol{u}^{(2)T}\boldsymbol{u}^{(1)}$$

$\boldsymbol{0} = (\lambda_1 - \lambda_2)\boldsymbol{u}^{(2)T}\boldsymbol{u}^{(1)}$ 兩式相減：

右式兩本徵向量的內積必須為零，彼此正交！

$\boldsymbol{u}^{(2)T}\boldsymbol{u}^{(1)} = \boldsymbol{u}^{(2)}\cdot\boldsymbol{u}^{(1)} = 0$ 本徵向量的正交性

證明：Prove Orthogonality!

$\hat{A}$作用於右邊的u_m，等於本徵值λ_m相乘。

$$\int_a^b dx \cdot u_n(x)^* \cdot \hat{A}u_m(x) = \lambda_m \int_a^b dx \cdot u_n(x)^* \cdot u_m(x)$$

$$= \int_a^b dx \cdot \left\{u_n^* \frac{d}{dx}\left[p(x)\frac{d}{dx}\right]u_m + q(x)u_n^* u_m\right\}$$

$$= \int_a^b dx \cdot \left\{-p\frac{du_n^*}{dx}\frac{du_m}{dx} + qu_n^* u_m\right\} + \left(u_n^*\left[p\frac{du}{dx}\right]\right)\Big|_a^b$$

$$= \int_a^b dx \cdot \left\{\frac{d}{dx}\left[p\frac{du_n^*}{dx}\right]u_m + qu_n^* u_m\right\} + \left(\left[p\frac{du_n^*}{dx}\right]u_m\right)\Big|_a^b$$

$$\lambda_n^* = \lambda_n$$

$$= \int_a^b dx \cdot \left\{\frac{d}{dx}\left[p\frac{du_n^*}{dx}\right] + qu_n^*\right\}u_m = \int_a^b dx \cdot [\hat{A}u_n]^* u_m = \lambda_n \int_a^b dx \cdot u_n(x)^* u_m(x)$$

等於$\hat{A}$作用於左邊的u_m，等於本徵值λ_m相乘。

$$(\lambda_m - \lambda_n)\int_a^b dx \cdot u_n(x)^* \cdot u_m(x) = 0$$

$$\lambda_m \neq \lambda_n$$

$$\int_a^b dx \cdot u_n(x)^* \cdot u_m(x) = 0$$

以上證明用到算子$\hat{A}$的這個性質：

$$\int_a^b dx \cdot u_n(x)^* \cdot \hat{A} u_m(x) = \int_a^b dx \cdot \left[\hat{A} u_n(x)\right]^* u_m(x)$$

這是對任意兩函數ϕ, ψ都對：

$$\int_a^b dx \cdot \left\{\phi^* \left[p \frac{d}{dx}\right] \psi + q\phi^* \psi\right\} = \int_a^b dx \cdot \left\{\frac{d}{dx}\left[p \frac{d\phi^*}{dx}\right] + q\phi^*\right\} \psi$$

具有這樣性質的算子稱為Hermitian：

Hermitian算子的本徵值永遠是實數!

Hermitian算子不同本徵值的本徵函數彼此正交!

Charles Hermite 1822-1901

現在開始完備性的證明！The proof of the completeness.

若確認任一合邊界條件的函數可以本徵函數分解，我們就能計算其分解係數a_n。

但這樣的分解真的是正確的嗎？分解所得的無限級數真的與被分解的函數相等嗎？

數學上相等與否的判準：這些係數組成的u_n的線性組合，會趨近被分解的函數。

$$\lim_{N\to\infty}\int_0^L dx\left[\psi(x)-\sum_{n=1}^{N}a_n u_n(x)\right]^2=0$$

兩者差距的平方和(積分)$N\to\infty$時，趨近於零。

這稱為Completeness.完備性，必須嚴格證明的。下學期將說明。

Sturm-Liouville Problem

$$\hat{A} \cdot u_n(x) = \frac{d}{dx}\left[p(x)\frac{d}{dx}u_n(x)\right] + q(x)u_n(x) = \lambda_n \cdot u_n(x)$$

Under boundary conditions, the equation has a countable set of solutions.

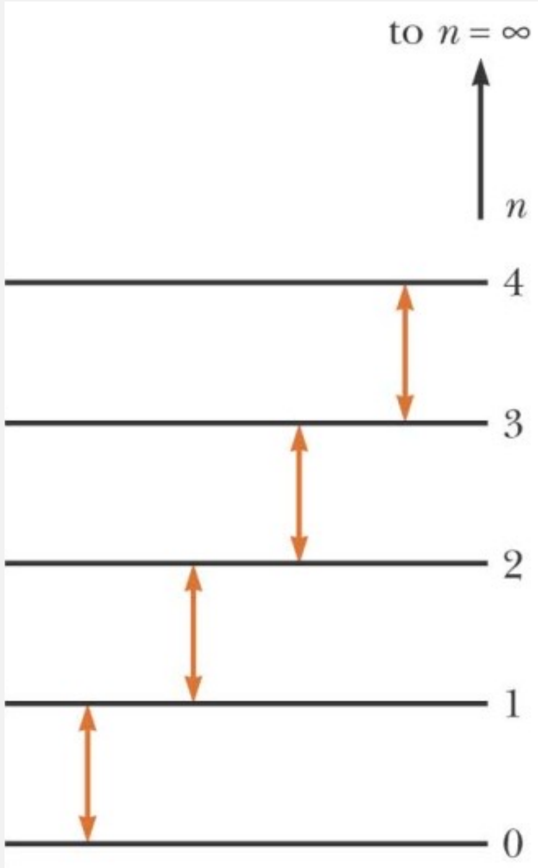
We can classify them by n and order them by eigenvalues from small to large:

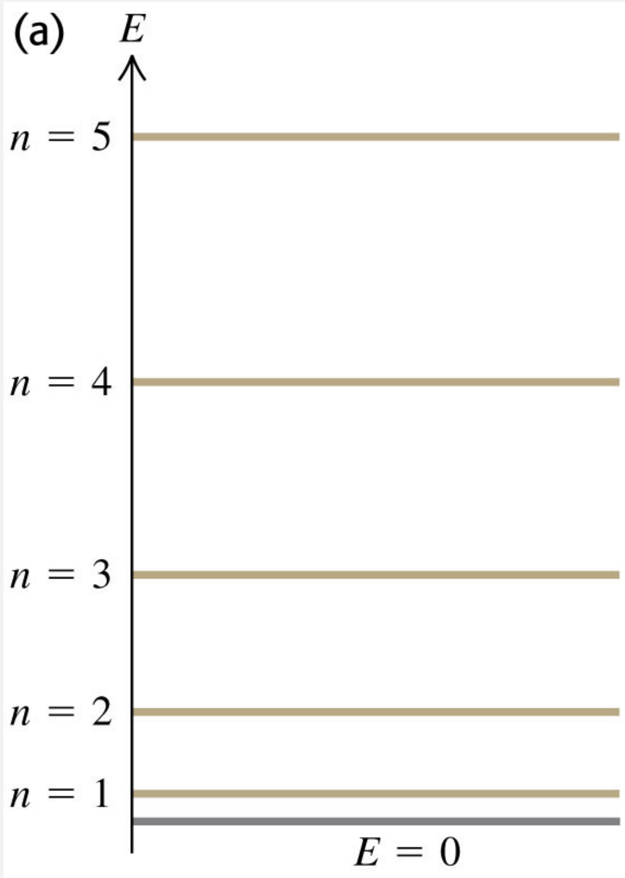
$$\lambda_1 < \lambda_2 < \cdots < \lambda_n < \cdots$$

It could be proven that λ_n is unbounded: $\lambda_n \to \infty, \text{as } n \to \infty$

We'll skip the proof of this crucial step since it's too technical.

But it is reasonable and true for the examples we talked about.





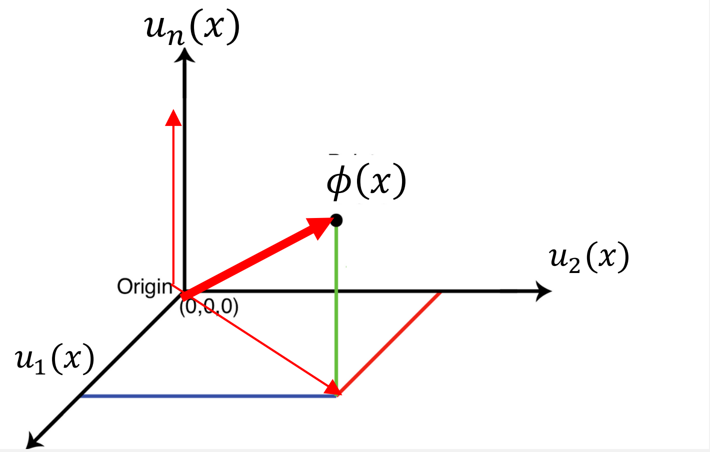
$\lambda_1 < \lambda_2 < \cdots < \lambda_n < \cdots$ 每一個本徵值λ_n對應一個函數$u_n(x)$，

$\lambda_1 < \lambda_2 < \cdots < \lambda_n < \cdots$ 每一個本徵值λ_n對應一個函數$u_n(x)$，

用向量的類比，每一個$u_n(x)$都是一個彼此正交單位向量，展開一維的空間：

$u_n(x)$是一個彼此正交歸一的座標系統，直覺是：任一函數可以以此展開！

$$\psi(x) = \sum_{n=1}^{\infty} [a_n u_n(x)]$$



這個可以嚴格證明的數學性質稱為：$u_n(x)$是完備的complete。

展開定理：任一狀態函數ψ可以此$\hat{A}$本徵函數$u_n(x)$作分量展開。

$$\psi(x) = \sum_{n=1}^{\infty} [a_n u_n(x)]$$

若是分量展開是可能的，那分量c_a可以寫成：

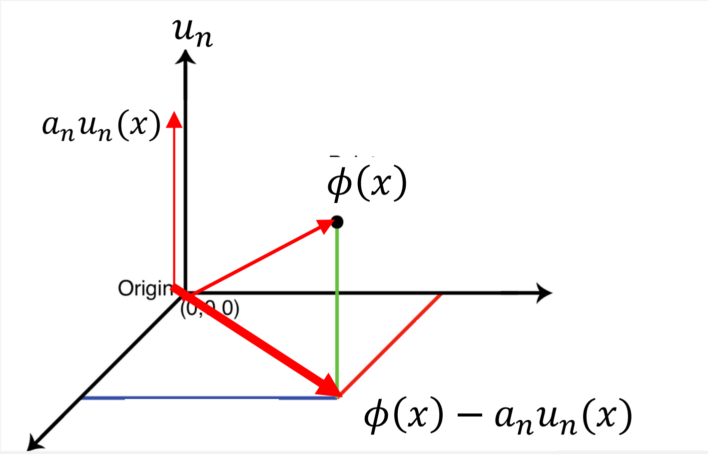
$$a_n = \int_a^b dx \cdot u_n(x)^* \cdot \psi(x)$$

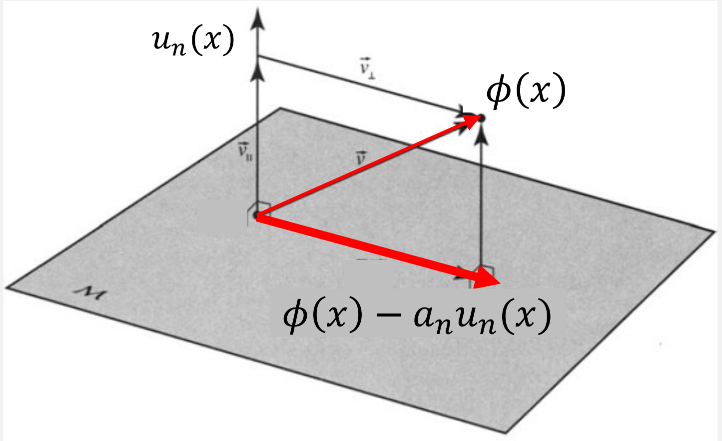
所以要證明的是：用如此分量c_a寫成的級數，會趨近正確的狀態函數：

$$\sum_{i=1}^{n} [a_i u_i(x)] \xrightarrow[n\to\infty]{} \psi(x)$$

趨近的數學判準之一，兩者差距的平方和(積分)$N \to \infty$時，趨近於零。

$$\lim_{n\to\infty} \int_a^b dx \left[\phi(x) - \sum_{i=1}^{n-1} a_i u_i(x)\right]^2 = 0$$





每一個$u_n(x)$都是一個彼此正交單位向量，展開一維的空間：

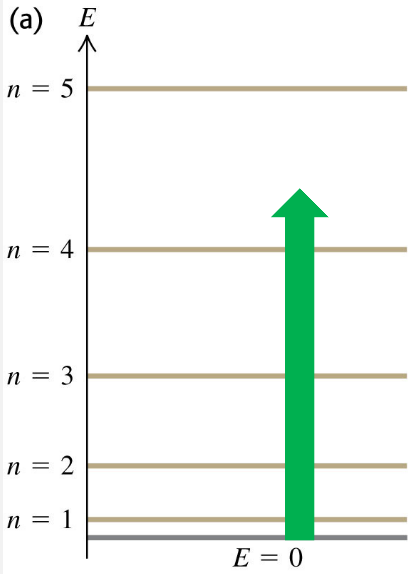
任一函數$\phi(x)$，投影在向量$u_n(x)$方向的分量可以算

$$a_n = \int_a^b dx \cdot u_n(x)^* \cdot \phi(x)$$

函數$\phi(x)$扣掉此投影後，就與$u_n(x)$的正交：$\phi(x) - a_n u_n(x)$

$$\langle u_n, [\phi - a_n u_n] \rangle = \int_{-\infty}^{\infty} dx \cdot u_n(x)^* \cdot [\phi(x) - a_n u_n(x)] = 0$$

扣掉投影$a_n u_n$的動作，壓縮此函數的空間，使只能存在於與u_n正交的平面上。



我們可以由下而上，一層一層將一函數$\phi(x)$的投影$a_i u_i$扣掉， ，

$$g_{n-1}(x) \equiv \phi(x) - \sum_{i=1}^{n-1} a_i u_i(x)$$

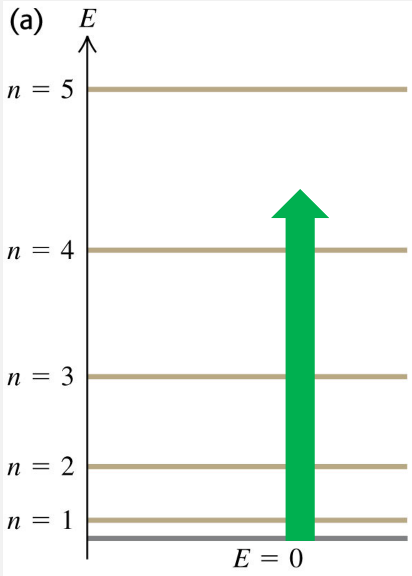
結果與N以下所有的向量$m < n$都正交：

$$\langle u_m, g_{n-1} \rangle = \int_a^b dx \cdot u_m(x)^* \cdot \left[\phi(x) - \sum_{i=1}^{n-1} a_i u_i(x) \right] = 0$$

如此函數被壓縮於"越來越高、越來越小"的空間中，直覺是向量長度會越來越短。

$$\lim_{n\to\infty} |g_{n-1}|^2 = \lim_{n\to\infty} \int_a^b dx \left[\phi(x) - \sum_{i=1}^{n-1} a_i u_i(x) \right]^2 =?\, 0$$

這正是完備性的數學判準，函數與其展開的差距的平方積分$n \to \infty$時，趨近於零。



$g_{n-1}(x)$就是函數$\phi(x)$、與其展開的有限級數之間的差距：

$$g_{n-1}(x) \equiv \phi(x) - \sum_{i=1}^{n-1} a_i u_i(x)$$

$g_{n-1}(x)$函數$n \to \infty$時，會被壓縮於越來越高、越來越限縮的空間中 ，

$g_{n-1}(x)$函數的集合，也就是這個越來越限縮的空間，給個符號V_{n-1}

注意$u_m, m < n$不在這空間中，因為$g_{n-1}(x)$與他們都正交。

當$n \to \infty$，$g_{n-1}(x)$函數被壓縮於越來越小、越來越限縮的空間V_{n-1}，何謂越來越小、越來越限縮的空間？

將證明，在此空間中的向量$g_{n-1}(x)$，其向量長度小於本徵值的倒數：

$$|g_{n-1}|^2 < \frac{c}{\lambda_n}$$

已知：

$$\lambda_n \to \infty, \text{as } n \to \infty$$

因此：

$$\lim_{n \to \infty} |g_{n-1}|^2 \to 0$$

Rayleigh quotient 瑞利之商

對任一函數$u(x)$，S-L算子$\hat{A}$，可以定義一個商：

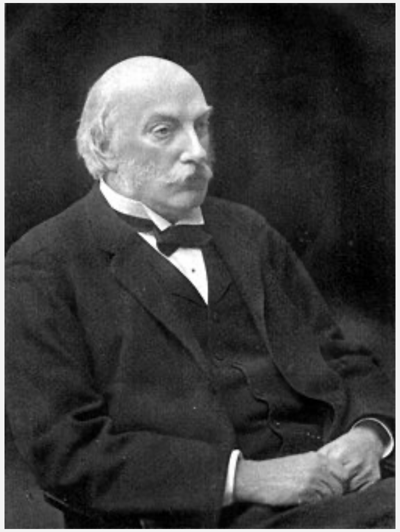
$$R[u] = \frac{\langle u, \hat{A}u \rangle}{|u|^2}$$

定理一：

瑞利之商的極值就是$\hat{A}$的本徵值，發生在本徵函數時。

瑞利之商的最小值就是$\hat{A}$的最小本徵值λ_1。

最小值發生時的函數u就是本徵值λ_1對應的本徵函數u_1。



Lord Rayleigh 1842-1919

$$\lambda_1 \leq R[u] = \frac{\langle u, \hat{A}u \rangle}{|u|^2}$$

定理二：

若只對與$u_m, m < n$正交的$g_{n-1}(x)$算$R[g_{n-1}]$，最小值為次一個本徵值λ_n。

最小值發生時的函數u就是本徵值λ_n對應的本徵函數u_n。

$$\lambda_n \leq R[g_{n-1}] = \frac{\langle g_{n-1}, \hat{A}g_{n-1} \rangle}{|g_{n-1}|^2}$$

注意：

$$|g_{n-1}|^2 \leq \frac{\langle g_{n-1}, \hat{A}g_{n-1} \rangle}{\lambda_n}$$

若分子有限， $|g_{n-1}|^2 < \frac{c}{\lambda_n}$ $\lim_{n\to\infty} |g_{n-1}|^2 \to 0$ 完備性就得證了！

Rayleigh quotient 瑞利之商有一個很簡單性質：

對任一算子$\hat{A}$的本徵函數$u_n(x)$，

$$\hat{A} \cdot u_n = \lambda_n \cdot u_n$$

瑞利之商就等於其本徵值：

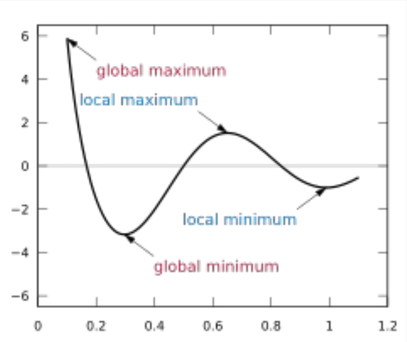
$$R[u_n] = \frac{\langle u_n, \hat{A} u_n \rangle}{|u_n|^2} = \frac{\langle u_n, \lambda_n u_n \rangle}{|u_n|^2} = \frac{\lambda_n \langle u_n, u_n \rangle}{|u_n|^2} = \lambda_n$$

$$R[u_n] = \lambda_n$$

定理一證明：

瑞利之商的極值可以用常見的極值計算法找：

極值之處斜率為零，極值附近函數圖形是平的：$\dfrac{df}{dx} = 0$

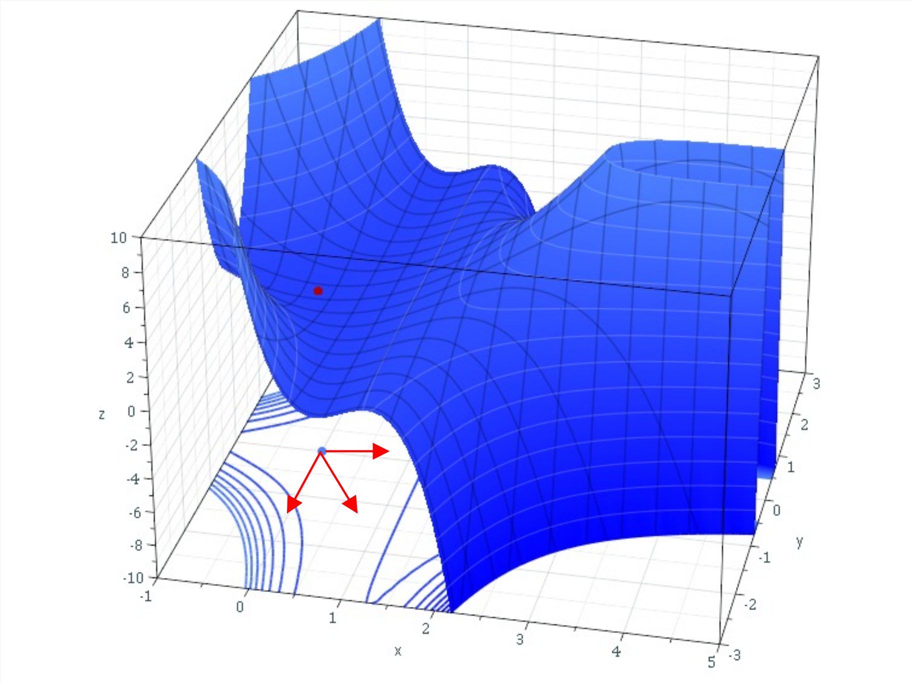


現在可變的量不是變數，而是函數。

但原理相同，極值是谷底，附近函數是平坦的。假設極值發生在某函數$u_*(x)$，

u_*加上任意一點小偏移deviation $tu(x)$：$u_*(x) + tu(x)$，變化率為零：

$$\frac{d}{dt} R[u_* + tu] = 0$$



$$\frac{d}{dt}R[u_* + tu] = 0$$

$$R[u] = \frac{\langle u, \hat{A}u \rangle}{|u|^2}$$

$$R[u_* + tu] = \frac{\langle (u_* + tu), \hat{A}(u_* + tu) \rangle}{|u_* + tu|^2}$$

$$= \frac{\langle u_*, \hat{A}u_* \rangle + 2t\langle u, \hat{A}u_* \rangle + t^2 \langle u, \hat{A}u \rangle}{|u_*|^2 + t^2|u|^2 + 2t\langle u, u_* \rangle}$$

注意：

$$\langle u_*, \hat{A}u \rangle = \langle \hat{A}u_*, u \rangle = \langle u, \hat{A}u_* \rangle$$

在$t = 0$取微分需為零：

$$\frac{dR[u_* + tu]}{dt}(t = 0) = \frac{2\langle u, \hat{A}u_* \rangle |u_*|^2 - 2\langle u_*, \hat{A}u_* \rangle \langle u, u_* \rangle}{|u_*|^4} = 0$$

$$\langle u, \hat{A}u_* \rangle |u_*|^2 - \langle u_*, \hat{A}u_* \rangle \langle u, u_* \rangle = 0$$

$$\langle u, \hat{A}u_* \rangle - \frac{\langle u_*, \hat{A}u_* \rangle}{|u_*|^2} \langle u, u_* \rangle = 0$$

$$\langle u, \hat{A}u_* \rangle - R[u_*] \langle u, u_* \rangle = 0$$

$$\langle u, \hat{A}u_* - R[u_*]u_* \rangle = 0$$

此式對任意$u(x)$都要成立，唯一可能：內積中的右邊必須為零！

$$\hat{A}u_* - R[u_*]u_* = 0$$

$R[u_*]$是一個數，因此瑞利之商的極值必須是本徵值！

$\hat{A}u_* - R[u_*]u_* = 0$ 瑞利之商的極值必須是本徵值 ！

而且極值發生的函數u_*就是本徵函數。

因為所有本徵函數的瑞利之商就等於其本徵值，

最小瑞利之商必須是最小的本徵值：λ_1！

而且極值發生的函數u_*就是本徵函數u_1。

$$\lambda_1 \leq R[u] = \frac{\langle u, \hat{A}u \rangle}{|u|^2}$$

定理一得證！

定理二：

若只對已扣掉n前面本徵函數投影的$g_{n-1}(x)$，計算瑞利之商$R[g_{n-1}]$，

最小值為次一個本徵值λ_n，發生時的函數u就是本徵值λ_n對應的本徵函數u_n。

$$\lambda_n \le R[g_{n-1}]$$

證明：如定理一，最小值一定是一個本徵值。

n前面本徵函數$u_m, m < n$都不是$g_{n-1}(x)$，因為所有$g_{n-1}(x)$都與 $u_m, m < n$正交。

最小的瑞利之商$R[g_{n-1}]$只能是下一個本徵值：λ_n。

$$\lambda_n \le R[g_{n-1}]$$

定理二得證！

現在只剩最後一步：
$$\lambda_n \le R[g_{n-1}] = \frac{\langle g_{n-1}, \hat{A} g_{n-1}\rangle}{|g_{n-1}|^2}$$

注意：
$$|g_{n-1}|^2 \le \frac{\langle g_{n-1}, \hat{A} g_{n-1}\rangle}{\lambda_n}$$

$$\langle g_{n-1}, \hat{A} g_{n-1}\rangle = \left\langle \left(\phi(x) - \sum_{i=1}^{n-1} a_i u_i(x)\right), \hat{A}\left(\phi(x) - \sum_{i=1}^{n-1} a_i u_i(x)\right)\right\rangle$$

$$= \langle \phi, \hat{A}\phi\rangle - \left\langle \phi, \sum_{i=1}^{n-1} a_i \hat{A} u_i \right\rangle - \left\langle \sum_{i=1}^{n-1} a_i u_i \, , \hat{A}\phi \right\rangle + \sum_{j=1}^{n-1}\sum_{i=1}^{n-1} a_j^* a_i \langle u_j, \hat{A} u_i\rangle$$

$$= \langle \phi, \hat{A}\phi\rangle - \left\langle \phi, \sum_{i=1}^{n-1} a_i \hat{A} u_i \right\rangle - \left\langle \sum_{i=1}^{n-1} a_i \hat{A} u_i \, , \phi \right\rangle + \sum_{j=1}^{n-1}\sum_{i=1}^{n-1} a_j^* a_i \lambda_i \langle u_j, u_i\rangle$$

$$= \langle \phi, \hat{A}\phi\rangle - \sum_{i=1}^{n-1} a_i \lambda_i \langle \phi, u_i\rangle - \sum_{i=1}^{n-1} a_i^* \lambda_i \langle u_i, \phi\rangle + \sum_{j=1}^{n-1}\sum_{i=1}^{n-1} a_j^* a_i \lambda_i \delta_{ij}$$

$$= \langle \phi, \hat{A}\phi\rangle - \sum_{i=1}^{n-1} a_i^* a_i \lambda_i - \sum_{i=1}^{n-1} a_i^* a_i \lambda_i + \sum_{i=1}^{n-1} a_i^* a_i \lambda_i = \langle \phi, \hat{A}\phi\rangle - \sum_{i=1}^{n-1} a_i^* a_i \lambda_i < \langle \phi, \hat{A}\phi\rangle$$

$$|g_{n-1}|^2 \leq \frac{\langle g_{n-1}, \hat{A} g_{n-1} \rangle}{\lambda_n} < \frac{\langle \phi, \hat{A}\phi \rangle}{\lambda_n}$$

分子是有限值！

$$\lim_{n\to\infty} |g_{n-1}|^2 \to 0$$

$$g_{n-1}(x) \equiv \phi(x) - \sum_{i=1}^{n-1} a_i u_i(x)$$

$g_{n-1}(x)$：函數$\phi(x)$、與其展開的有限級數之間的差距趨近於零！

Sturm-Liouville 算子本徵函數的完備性就得證了！

任何位能薛丁格波方程式都是S-L方程式，之前的普遍解法一率適用：

將$t=0$時的波函數，即起始條件，對定態解u_n展開如下：

$$\Psi(x,0)=\sum_{n=1}^{\infty}c_n u_n(x)$$

根據展開定理，這永遠可以做到！

$t=0$時此狀態可以視為定態u_n的如上疊加，

接著定態隨時間個自演化，位能下薛丁格方程式要求u_n乘上$e^{-i\frac{E_n}{\hbar}t}$。

乘完之後依同樣方式疊加，整個波函數也就滿足薛丁格波方程式。

$$\Psi(x,t)=\sum_{n=1}^{\infty}c_n u_n(x)e^{-i\frac{E_n}{\hbar}t}$$

很明顯，這個程序不只適用於無限大位能井，原則上適用於任何位能。