

LaTeX Typesetting By Example

Phil Farrell

Stanford University School of Earth Sciences

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$$-\hbar^2/(2m)\nabla^2\psi = i\hbar\partial_t\psi$$

$$\psi_p(x) = e^{i/\hbar(px-p^2/(2m)t)}$$

$$\Psi(x) = \int dp \phi_x(p) \psi_p(x)$$

Note

$$\int dx \psi_p^*(x) \psi_p(x) = e^{i/\hbar((p'^2-p^2)/(2m)t)} 2\pi\delta(1/\hbar(p-p')) = 2\pi\hbar\delta(p-p')$$

$$\phi_x(p) = \frac{1}{2\pi\hbar} \int dx \psi_p^*(x) \Psi(x)$$

the solution for any time:

$$\Psi(x, t) = \int dp \frac{1}{2\pi\hbar} \int dy \psi_p^*(y) \Psi(y) \psi_p(x, t)$$

$$\Psi(x, t) = \int dy \Psi(y) \int dp \frac{1}{2\pi\hbar} \psi_p^*(y) \psi_p(x, t)$$

$$\Psi(x, t) = \int dy \Psi(y) \int dp \frac{1}{2\pi\hbar} e^{i(p(x-y)/\hbar - p^2 t/(2m\hbar))}$$

$$T = t/(m\hbar)$$

$$\Psi(x,t) = \int dy \Psi(y) \frac{1}{2\pi\hbar} (1-i) e^{i(x-y)^2/(2T\hbar^2)} \sqrt{\pi/T}$$

For space a

$$-\hbar^2/(2ma^2)(\psi(x+a)+\psi(x-a)-2\psi(x))\psi=i\hbar\partial_t\psi$$

$$\psi_p(x)=e^{i/\hbar(px-\hbar^2(1-\cos(ap/\hbar))/(ma^2)t)}$$

$$\psi_p(x)=e^{i/\hbar(px-(p^2/(2m))t)}$$

$$0\leq p<2\pi/a$$

$$\sum_{x_i}\psi_{p'}^*(x_i)\psi_p(x_i)=e^{i/\hbar(\hbar^2(1-\cos(ap'/\hbar)-\hbar^2(1-\cos(ap/\hbar))/(ma^2)t)}\sum_{x_i}e^{i(p-p')x_i/\hbar}=2\pi\delta(1/\hbar(p-p'))$$

$$x_i=ai$$

$$\phi_x(p)=\frac{1}{2\pi\hbar}\sum_{x_i}\psi_p^*(x_i)\Psi(x_i)$$

$$\Psi(x,t)=\sum_{y_i}\Psi(y_i)\int dp\frac{1}{2\pi\hbar}e^{ip(x-y)/\hbar-i\hbar(1-\cos(ap/\hbar))/(ma^2)t}$$

$$g(k)=\int dx f(x)\exp(ikx)$$

$$f(x)=\frac{1}{2\pi}\int dk g(k)\exp(-ikx)$$

$$f(x)=\sum_j\delta(x-ja)$$

$$g(k)=\int dx\sum_j\delta(x-ja)\exp(ikx)=\sum_j\exp(ijka)$$

$$f(x)=\sum_j\delta(x-ja)=\frac{1}{2\pi}\int dk g(k)\exp(-ikx)$$

$$g(k)=1/(2\pi a)\sum_n\delta(k+2\pi n/a)$$

1 Infinite Wall

Eigen state

$$\psi_k(j) = \sin(jk\pi/N)$$

$$j = 0..N - 1$$

$$k = 1..N - 1$$

Eigen value

$$E_k = k\pi/(Na)$$

$$\sum_j \psi_j(k) \psi_j(k) = N/2$$

$$\Psi(j) = \sum_{k=1}^{N-1} \Phi(k) \psi_k(j)$$

$$\Phi(k) = (2/N) \sum_j \Psi(j) \psi_k(j)$$

$$\Phi(k) = (2/N) \sum_j \Psi(j) \sin(jk\pi/N)$$

$$\Phi(k) = (1/(Ni)) \sum_j \Psi(j) (\exp(ijk\pi/N) - \exp(-ijk\pi/N))$$

$$\Phi(k) = (1/(Ni)) \sum_j \Psi(j) (\exp(ijk2\pi/2N) - \exp(i(2N-j)k2\pi/2N))$$

$$\Phi(k) = \frac{1}{Ni} \left(\sum_j^{N-1} \Psi(j) \exp(ijk2\pi/2N) - \sum_{N+1}^{2N} \Psi(2N-j) \exp(jk2\pi/2N) \right)$$

by define

$$\Phi(N) = 0$$

$$\Phi(k) = \frac{1}{Ni} \left(\sum_j^{N-1} \Psi(j) \exp(ijk2\pi/2N) - \sum_{j=N}^{2N-1} \Psi(2N-j) \exp(ijk2\pi/2N) \right)$$

$$\Phi(k) = \frac{1}{Ni} \left(\sum_{j=0}^{2N-1} \Psi'(j) \exp(ijk2\pi/2N) \right)$$

$$\Psi'(j) = \Psi(j) (j \leq N-1)$$

$$\Psi'(j) = 0 (j = N)$$

$$\Psi'(j) = -\Psi(2N-j) (j > N)$$

$$\Phi(k) = \frac{1}{Ni} \text{invfft}(2N, \Psi'(j), k)$$

$$\Psi(j) = \sum_{k=1}^{N-1} \Phi(k) \sin(jk\pi/N)$$

$$\Psi(j) = \frac{1}{2i} \text{invfft}(2N, \Phi'(k), j)$$

2 Split Method

Second order approximation

$$e^{t+v} = e^{1/2v} e^t e^{1/2v}$$

Fourth-order approximation

$$e^{t+v} = e^{c_1v} e^{d_1t} e^{c_2v} e^{d_2t} e^{c_2v} e^{d_1t} e^{c_1v}$$

where

$$c_1 = 1/(2(2 - 2^{1/3}))$$

$$c_2 = (1 - 2^{1/3})/(2(2 - 2^{1/3}))$$

$$d_1 = 1/(2 - 2^{1/3})$$

$$d_2 = -2^{1/3}/(2 - 2^{1/3})$$

3 Eigen Method

4 Gauss-Legendre Method

The SE, can be written as

$$\frac{d\psi}{dt} = -Ih\psi$$

the formal solution is

$$\psi(t) = e^{-Iht}\psi(0)$$

In numerical analysis, many methods are special cases of Runge-Kutta methods.

- Euler Method
 - Forward Euler Method
 - Backward Euler Method
- Gauss-Legendre Method
- ...

4.1 Forward euler method

$$\psi(t + \Delta t) = (1 - I\Delta th)\psi(t)$$

In numerical methods two things we should take care of:

- the local time discrete error
- the numerical stability, numerical stability means the result are bounded

For the Forward euler method, the local time discrete error is $O(\Delta t^2)$

$$\psi(t + \Delta t) = (1 - I\Delta th)\psi(t) + O(\Delta t^2)$$

We say this method is order One.

Numerical stability requires

$$|(1 - I\Delta th)\psi(t)| < (1 + \epsilon)|\psi(t)|$$

For every $\psi(t)$. for ϵ we need

$$(1 + \epsilon)^{T/\Delta t} - 1 \ll 1$$

or

$$\epsilon \ll \Delta t/T$$

we have

$$|(1 - I\Delta th)\psi(t)| < (1 + \Delta t/T)|\psi(t)|$$

For a eigenstate of eigenenergy of e , we have

$$|1 - I\Delta te| \leq (1 + \Delta t/T)$$

$$(\Delta te)^2 \leq 2\Delta t/T$$

Because $T \gg \Delta t$, so

$$(\Delta te)^2 \ll 1$$

For a discrete eystem. the max energy is $\hbar^2/2m/(\Delta x)^2$. So we need

$$\Delta t < (\hbar^2/2m(\Delta x)^2)^{-1}$$

The requirement for Δt is too strict.

4.2 Backward Euler method

$$\psi(t + \Delta t) = (1 + I\Delta th)^{-1}\psi(t)$$

This is an order of One method The stability requires

$$|(1 + I\Delta th)^{-1}\psi| < (1 + \Delta t/T)\psi$$

Because for each eigenstate with eigenernery of e

$$|(1 + I\Delta te)^{-1}| < 1 < (1 + \Delta t/T)$$

This methods is unconditional stable

4.3 Gauss-Legendre methods

Gauss-Legendre methods are implicit Runge-Kutta methods.

The Gauss-Legendre method of order two is also called implicit midpoint method. We don't describe the details of Gauss-Legendre Methods. We only conclude some key points here.

$$k_1 = -Ih(t_1)(1 + c_{11}k_1\Delta t + c_{12}k_2\Delta t)$$

$$k_2 = -Ih(t_2)(1 + c_{21}k_1\Delta t + c_{22}k_2\Delta t)$$

$$\psi(t + \Delta t) = (1 + k_1\Delta t + k_2\Delta t)\psi(t)$$

k_1 is solved as

$$k_1 = A_1(1 - c_{22}A_2\Delta t - c_{11}A_1\Delta t + (c_{22}c_{11} - c_{12}c_{21})A_1A_2(\Delta t)^2)^{-1}(1 + (-c_{22} + c_{12})A_2\Delta t)$$

$$k_2 = A_2(1 - c_{22}A_2\Delta t - c_{11}A_1\Delta t + (c_{22}c_{11} - c_{12}c_{21})A_2A_1(\Delta t)^2)^{-1}(1 + (-c_{11} + c_{21})A_1\Delta t)$$

where $A_i = -Ih(t_i)$.

When h is time independent the evolution is simplified as:

$$\psi(t + \Delta t) = (1 + 1/2I\Delta th)^{-1}(1 - 1/2I\Delta th)\psi(t)$$

$$\psi(t + \Delta t) = \frac{1 - 1/2I\Delta th - 1/12(\Delta th)^2}{1 + 1/2I\Delta th - 1/12(\Delta th)^2}\psi(t)$$

$$\psi(t + \Delta t) = \frac{1 - 1/2I\Delta th - 1/10(\Delta th)^2 + 1/120I(\Delta th)^3}{1 + 1/2I\Delta th - 1/10(\Delta th)^2 - 1/120I(\Delta th)^3}\psi(t)$$

Order of two method. Stable unconditionally. The transform each step is unitary matrix, so that the probability and energy are conserved.

5 Perturbation

The fermi golden rule

$$\Gamma_{i \rightarrow f} = \frac{2\pi}{\hbar} \rho_E |\langle \psi_f | V | \psi_i \rangle|^2$$

5.1 3D damental

In 3D,

$$\rho_E = \frac{\frac{V}{(2\pi\hbar)^3} p^2 d\Omega dp}{\frac{p dp}{m}} = \frac{mV}{(2\pi\hbar)^3} p d\Omega$$

Box normalization:

$$\psi_i(r) = \frac{1}{\sqrt{V}} e^{ik_i r}$$

$$\psi_i(r) = \frac{1}{\sqrt{V}} e^{ik_f r}$$

$$\langle \psi_f | V(r) | \psi_i \rangle = \frac{1}{V} \int dr V(r) e^{i(k_f - k_i)r}$$

$$\Gamma_{i \rightarrow f} = \frac{m p d\Omega}{(2\pi\hbar^2)^2 V} \left| \int dr V(r) e^{i(k_f - k_i)r} \right|^2$$

$$\Gamma_{i \rightarrow f} = \frac{d\sigma}{d\Omega} \frac{p}{m} |\psi_i|^2 d\Omega$$

$$\frac{d\sigma}{d\Omega} = \frac{m^2}{(2\pi\hbar^2)^2} \left| \int dr V(r) e^{i(k_f - k_i)r} \right|^2$$

For $V(r) = V_0 e^{-\alpha r^2}$

$$\int dr V(r) e^{i(k_f - k_i)r} = V_0 \left(\frac{\pi}{\alpha}\right)^{3/2} e^{-(k_i - k_f)^2 / (4\alpha)}$$

5.2 2D damental

In 2D,

$$\rho_E = \frac{\frac{V}{(2\pi\hbar)^2} p d\Omega dp}{\frac{p dp}{m}} = \frac{mV}{(2\pi\hbar)^2} d\Omega$$

Box normalization:

$$\psi_i(r) = \frac{1}{\sqrt{V}} e^{ik_i r}$$

$$\psi_i(r) = \frac{1}{\sqrt{V}} e^{ik_f r}$$

$$\langle \psi_f | V(r) | \psi_i \rangle = \frac{1}{V} \int dr V(r) e^{i(k_f - k_i)r}$$

$$\Gamma_{i \rightarrow f} = \frac{md\Omega}{2\pi\hbar^3 V} \left| \int dr V(r) e^{i(k_f - k_i)r} \right|^2$$

$$\Gamma_{i \rightarrow f} = \frac{d\sigma}{d\Omega} \frac{p}{m} |\psi_i|^2 d\Omega$$

$$\frac{d\sigma}{d\Omega} = \frac{m^2}{2\pi\hbar^3 p} \left| \int dr V(r) e^{i(k_f - k_i)r} \right|^2$$

For $V(r) = V_0 e^{-\alpha r^2}$

$$\int dr V(r) e^{i(k_f - k_i)r} = \frac{V_0 \pi}{\alpha} e^{-(k_i - k_f)^2 / (4\alpha)}$$