LaTeX Typesetting By Example

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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:

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

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

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

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

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

For space a

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

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

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

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

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

$$x_i = ai$$

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

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

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

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

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

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

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

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

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

$$e^{t+v} = e^{c_1 v}e^{d_1 t}e^{c_2 v}e^{d_2 t}e^{c_2 v}e^{d_1 t}e^{c_1 v}$$

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 $O(\Delta^2 t)$

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

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

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

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 $T >> \Delta t$, so

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

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 requrement 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 requres

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

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 decribe the details of Gauss-Legendre Methods. We only conclude some key points here.

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

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

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

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