Tuesday, February 9, 2021 15:04

$$f''(x_i) = \frac{f_{i+1} - 2f_i + f_{i-1}}{\Delta x^2}$$

$$f''\left(\frac{L}{2}\right) = \emptyset \Rightarrow$$

$f(x_i) = f_i, \quad i = \emptyset, 1, \dots$ $\qquad -1 \ \emptyset \ 1 \ 2 \ 3 \ \dots$

$$x_i = -\frac{L}{2} + i\frac{L}{N-1}$$

p.b.c $f'_\emptyset = \emptyset$ $\qquad f'(x_i) = \frac{f_{i+1} - f_{i-1}}{2\Delta h}$

$$f'(x_0) = \frac{f_1 - f_{-1}}{2\Delta h} = \emptyset$$

$$\boxed{f_{-1} = f_1}$$

z.b.c $f_{-1} = \emptyset$

$$\Delta \rightarrow \begin{pmatrix} -2; & 1 \rightarrow 2 & \\ 1; & -2; & 1 \\ & 1; & -2; \ 1 \\ & & \ddots \end{pmatrix}$$

p.b.c $f''_\emptyset = \frac{f_1 - 2f_0 + f_{-1}}{2\Delta x^2} = \frac{2f_1 - 2f_0}{2\Delta x^2}$

$$\frac{\hbar^2}{2m}\left(-\frac{\partial^2}{\partial x^2} - \frac{\partial^2}{\partial y^2}\right) f(x,y) = E f(x,y)$$

$$f(x,y) = f(x)\, f(y)$$

$$\frac{\hbar^2}{2m}\left(-\frac{\partial^2}{\partial x^2}\right) f(x) = E_x f(x)$$

$$\text{11-11} \qquad = E_y$$

$$= E_x f(x) f(y) + E_y f(x) f(y)$$

$$= (E_x + E_y)\, f(x,y)$$

$$E = E_x + E_y \underset{\text{g.s.}}{=} 2E_x$$

$$-\frac{\hbar^2}{2m} f''(x) = E_x f(x)$$

$$f(x) = A\sin(kx) + B\cos(kx)$$

$$f'(x) = Ak\cos(kx) - Bk\sin(kx)$$

$$f(x) = A\sin(kx) + B\cos(kx)$$

$$f'(x) = Ak\cos(kx) - Bk\sin(kx)$$

$$f''(x) = -Ak^2 \sin kx - Bk^2 \cos kx$$

$$= -k^2 f(x)$$

$$\frac{\hbar^2 k^2}{2m} = E_x$$

Free parameters A, B, k

Boundary condition.

a) p.b.c $\quad f'\left(\frac{L}{2}\right) = 0$

$$\Rightarrow k = 0 \quad ; \quad \boxed{f(x) = B \cdot \cos 0x = B = \text{Const}}$$

$$\boxed{E = \frac{\hbar^2 k^2}{2m} = 0}$$

b) z.b.c. $\quad f\left(\frac{L}{2}\right) = 0$

$$f\left(-\frac{L}{2}\right) = 0$$

$$f\left(\frac{L}{2}\right) = A\sin\frac{kL}{2} + B\cos\frac{kL}{2} = 0$$

$$f\left(-\frac{L}{2}\right) = -A\sin\frac{kL}{2} + B\cos\frac{kL}{2} = 0$$

$$f\left(\frac{L}{2}\right) + f\left(-\frac{L}{2}\right) = 2B\cos\frac{kL}{2} = 0$$

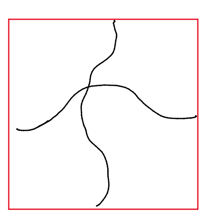
$$\frac{kL}{2} = \frac{\pi}{2}$$

$$k = \frac{\pi}{L}$$

$$E_x = \frac{\pi^2}{2m}\frac{\hbar^2}{L^2}$$

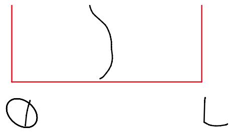
$$\boxed{E = \frac{\pi^2 \hbar^2}{mL^2}}$$

L



$$\begin{cases} f(x,y) = \sin\frac{\pi}{L}x \cdot \sin\frac{\pi}{L}y \\ f(x=0, y) = 0 \end{cases}$$

$$\begin{cases} f(x,y) = \sin \frac{\pi}{L} x \cdot \sin \frac{\pi}{L} y \\ f(x=0, y) = 0 \\ f(x=L, y) = \sin\pi \cdot \ldots = 0 \end{cases}$$



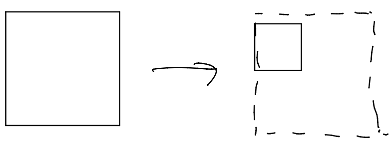
$$\boxed{f(x,y) = \sin \frac{\pi}{L}\left(x - \frac{L}{2}\right) \cdot \cos \frac{\pi}{2}\left(x - \frac{L}{2}\right)}$$

$$f\left(\frac{L}{2}, y\right) = \sin 0 \to 0$$

$$f\left(-\frac{L}{2}, y\right) = \sin \frac{\pi}{L}(-L) \cdot \ldots = \sin(-\pi) \ldots = 0$$

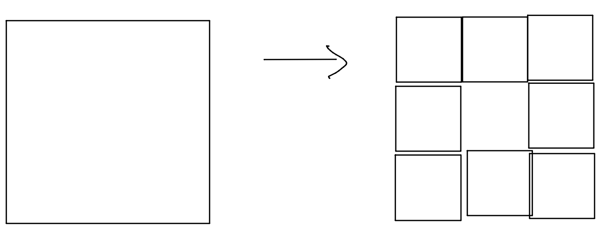
Energy upper bound:

1) iteration i : $\tilde{L} = \frac{L}{3^i}$



$$E = \pi^2 \frac{\hbar^2}{mL^2} \to \frac{\pi^2}{(1/3^i)^2} \frac{\hbar^2}{mL^2} = \pi^2 9^i \frac{\hbar^2}{mL^2}$$

2) Improved upper bound



iteration 1 $\quad N$ squares $\quad N = 8$

$$E = \pi^2 \frac{\hbar^2}{mL^2} = \pi^2 \frac{\hbar^2}{m} \frac{N_p}{L^2} = \pi^2 \frac{\hbar^2}{m} n$$

$n = \frac{N_p}{L^2}$ - density $\quad N_p \to$ number of particles

Iteration: $\quad N_{total} = 9 \quad\quad N_p = \sum_{occupied} \tilde{N}_p$

$N_{occupied} = 8 \quad\quad = N_{occupied} \cdot \tilde{N}_p$

$$\tilde{N}_p = \frac{N_p}{N_{occupied}}$$

$$\tilde{n}_p = \tilde{N}_p \ \_ \ \frac{N_p \quad 9^i}{\quad}$$

$$\tilde{n}_p = \frac{\overset{N_{occupied}}{\tilde{N}_p}}{\tilde{L}^2} = \frac{N_p \quad g^i}{N_{occupied} \quad L^2}$$

$$E = N_{occupied} \cdot \pi^2 \cdot \frac{\hbar^2}{m} \frac{N_p \cdot g^i}{N_{occupied} \cdot L^2}$$

$$= \pi^2 g^i \frac{\hbar^2}{mL^2}$$

Periodic boundary conditions

1D Box

$$\underbrace{-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} f(x)} = E f(x)$$

$$f(x) = e^{ikx}$$

$$f'(x) = ik e^{ikx}$$

$$f''(x) = (ik)^2 e^{ikx} = -k^2 f(x)$$

$$E = \frac{\hbar^2 k^2}{2m}$$

k?

p.b.c.: $f(L) = f(0)$

$$f(L) = e^{ikL} = f(0) = e^{ik0} = 1$$

$$e^{ikL} = 1 \qquad kL = 2\pi \cdot n, \quad n = 0; \pm 1; \pm 2, \ldots$$

$$k = \frac{2\pi}{L} \cdot n$$

$$E = \frac{\hbar^2 k^2}{2m} = \frac{2\pi^2}{mL^2} \cdot n^2$$

w.f

ground state: $n = 0$, $E_0 = 0$ $\qquad f_0(x) = 1$

1st excited state: $n = 1$; $E_1 = \frac{2\pi^2}{mL^2}$ $\qquad f_1(x) = e^{i\frac{2\pi}{L}x}$

2nd excited state $n = -1$ $E_2 = \frac{2\pi^2}{mL^2} = E_1$ $\qquad f_2(x) = e^{-i\frac{2\pi}{L}x}$

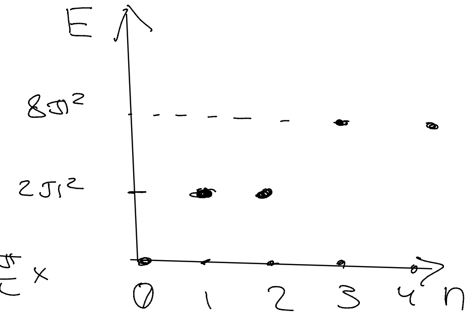
3rd $\quad n = 2$ $\qquad E_3 = E_4 = \frac{8\pi^2}{mL^2}$ $\qquad f_3(x) = e^{i\frac{4\pi}{L}x}$

4rd $\quad n = -2$ $\qquad f_4(x) = e^{-i\frac{4\pi}{L}x}$

$E \uparrow$

4ra $\qquad$ $\overline{mL^2}$ $\qquad$ $f_4(x)$

$n = -2$



$$\frac{f_1(x) + f_2(x)}{2} = \frac{e^{i\frac{2\pi}{L}x} + e^{-i\frac{2\pi}{L}x}}{2}$$

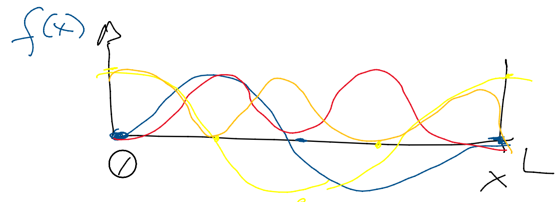
$$= \cos \frac{2\pi}{L} x$$

$$\frac{f_1(x) - f_2(x)}{2} = \frac{e^{i\frac{2\pi}{L}x} - e^{-i\frac{2\pi}{L}x}}{2}$$

$$= \sin \frac{2\pi}{L} x$$

$n(x) = f(x)^2$

$$f''(x) = -\frac{4\pi^2}{L^2} f(x)$$



$$\left(\sin \frac{2\pi}{L} x\right)^2$$

$$\left(\cos \frac{2\pi}{L} x\right)^2 \rightarrow n(x)$$

2D) $\quad -\frac{\hbar^2}{2m}\left[f''_{xx} + f''_{yy}\right] = E f(x,y)$

0) ground state: $f(x,y) = 1$

$E = 0$

1) 1^{st} excited state $\quad f(x,y) = \cos \frac{2\pi}{L} x$

$$f''_{xx} = -\left(\frac{2\pi}{L}\right)^2 \cos \frac{2\pi}{L} x$$

$$f''_{yy} = 0$$

$$E_1 = \frac{\hbar^2}{2m}\left(\frac{2\pi}{L}\right)^2 = 2\pi^2 \frac{\hbar^2}{mL^2}$$

2) 2^{nd} excited state $\quad f(x,y) = \sin \frac{2\pi}{L} x$

$E_2 = E_1$

3) $\quad E_3 = E_1 \qquad f(x,y) = \cos \frac{2\pi}{L} y$

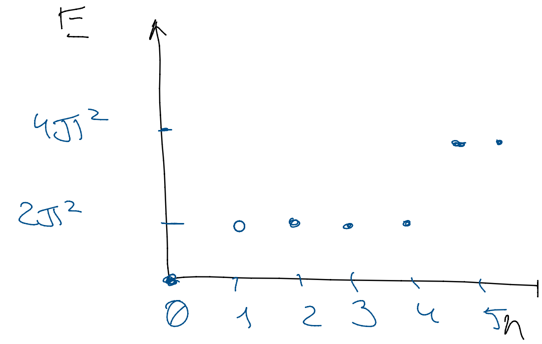
4) $\quad E_4 = E_1 \qquad f(x,y) = \sin \frac{2\pi}{L} y$

5) $\quad f(x,y) = \cos \frac{2\pi}{L} x \cdot \cos \frac{2\pi}{L} y$

$$E = \frac{\hbar^2}{2m}\left(\left(\frac{2\pi}{L}\right)^2 + \left(\frac{2\pi}{L}\right)^2\right) = 4\pi^2 \hbar^2$$

3) $f(x,y) = \cos\frac{2\pi}{L}x \cdot \cos\frac{2\pi}{L}y$

$E = \frac{\hbar^2}{2m}\left(\left(\frac{2\pi}{L}\right)^2 + \left(\frac{2\pi}{L}\right)^2\right) = 4\pi^2\frac{\hbar^2}{mL^2}$



Zero boundary condition

1D) $f(x) = Ae^{ikx} + Be^{-ikx}$

z.b.c: $f(0) = A + B = 0 \Rightarrow B = -A$

$f(L) = Ae^{ikL} + Be^{-ikL}$

$= Ae^{ikL} - Ae^{-ikL}$

$= A(e^{ikL} - e^{-ikL})$

$= A2\sin kL$

$\Rightarrow \sin kL = 0$

$kL = \pi n \quad , \quad n = 0; 1; 2 \ldots$

$= \pm\pi;\ \pm 3\pi;\ \pm 5\pi; \ldots$

as $\sin \pi\frac{x}{L}$ is the same as

$\sin\left(-\frac{\pi x}{L}\right)$, apart from sign,

only positive solutions are relevant

$\Rightarrow kL = \pi n \quad , \quad n = 1, 2 \ldots$

0) $n = 1;\quad \sin\frac{\pi}{L}x;\quad E = \frac{\pi^2}{2}\frac{\hbar^2}{m}\frac{\hbar^2}{mL^2}$

$n = 2;\quad \sin\frac{2\pi}{L}x;\quad E = 2\pi^2\frac{\hbar}{m}$

$$\frac{\quad}{2} \frac{\quad}{mL^2}$$

$n = 2;$ $\sin \frac{2\pi}{L} x$; $E = 2\pi^2 \frac{\hbar^2}{mL^2}$

3 $\frac{9}{2}\pi^2$

2D) $f(x,y) = \sin \frac{\pi}{L} n_x x \cdot \sin \frac{\pi}{L} n_y y$

$$E = \frac{\pi^2}{2}(n_x^2+n_y^2)\frac{\hbar^2}{mL^2} \quad ; n_x = 1,2,3,\ldots \quad n_y = 1,2,3\ldots$$

0) ground state ; $n_x = n_y = 1$

$$f(x,y) = \sin \frac{\pi}{L} x \cdot \sin \frac{\pi}{L} y$$

$$E = \pi^2 \frac{\hbar^2}{mL^2}$$

1st excited $n_x = 2$; $n_y = 1$

$$f(x,y) = \sin \frac{2\pi}{L} x \cdot \sin \frac{\pi}{L} y$$

$$E = \frac{5}{2}\pi^2 \frac{\hbar^2}{mL^2}$$

2st exc $f(x,y) = \sin \frac{\pi}{L} x \cdot \sin \frac{2\pi}{L} y$

$$E = \frac{5}{2}\pi^2 \frac{\hbar^2}{mL^2}$$

3st $n_x = n_y = 2$

$$f(x,y) = \sin \frac{2\pi}{L} x \cdot \sin \frac{2\pi}{L} y$$

$$E = 4\pi^2 \frac{\hbar^2}{mL^2}$$

Diffusion coefficient

Diffusion equation (single particle)

$$\begin{cases} -\frac{\partial}{\partial t} f(x,y,t) = -\frac{\hbar^2}{2m} \underbrace{\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right)}_{\text{kinetic energy}} f(x,y,t) \\ f(x,y,t=0) = \delta(\vec{r}). \end{cases}$$

Fourier transform: $FT[f(x)] = f(k)$

$(\quad f(x,y,t=0) = \delta(\ ) .$ kinetic energy

Fourier transform: $FT\left[f(x)\right] = f(k)$

$FT\left[\frac{\partial}{\partial x} f(x)\right] = k \cdot f(k)$

$FT\left[\frac{\partial^2}{\partial x^2} f(x)\right] = k^2 f(k)$

One-dimensional case:

$$\underbrace{\int e^{ikx} \frac{\partial}{\partial t} f(x,t) dx}_{\frac{\partial}{\partial t} \underbrace{\int e^{ikx} f(x,t) dx}_{f(k,t)}} = \frac{\hbar^2}{2m} \underbrace{\int \frac{\partial^2}{\partial x^2} f(x,t) \cdot e^{ikx} dx}$$

$$\cancel{\frac{\partial}{\partial x} f(x,t) \cdot e^{ikx} \Big|_{-\infty}^{\infty}} \to 0 - \int \frac{\partial}{\partial x} f(x,t) \cdot (ik) e^{ikx} dx$$

$$- \cancel{f(x,t)(ik) e^{ikx} \Big|_{-\infty}^{\infty}} \to 0 + \underbrace{\int f(x,t) \, (ik)^2 e^{ikx} dx}_{-k^2 f(k,t)}$$

$$\frac{\partial}{\partial t} f(k,t) = - \frac{\hbar^2 k^2}{2m} f(k,t)$$

$$f(k,t) = \exp\left\{ - \frac{\hbar^2 k^2}{2m} \cdot t \right\} \text{ - Gaussian}$$

D

momentum representation

Coordinate representation

$$f(x,t) = FT^{-1}\left[f(k)\right]$$

$$= \int_{-\infty}^{\infty} e^{-ikx} f(k) \frac{dk}{2\pi}$$

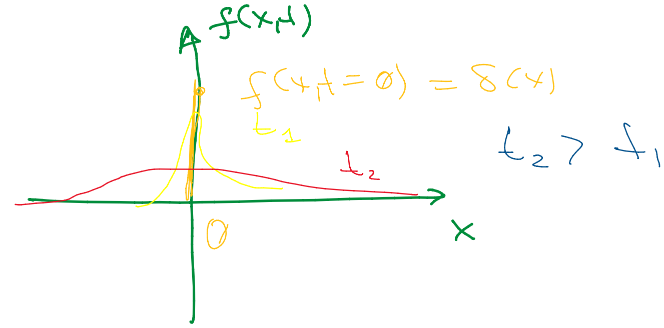
$$= \int_{-\infty}^{\infty} e^{-ikx} e^{-D \cdot k^2 \cdot t} \frac{dk}{2\pi}$$

$$= \frac{1}{2\sqrt{\pi D t}} \cdot \exp\left\{ - \frac{x^2}{4Dt} \right\} = \exp\left\{ -\frac{1}{2} \frac{x^2}{\sigma^2} \right\}$$

Gaussian of width $\sigma = \sqrt{2Dt}$

$f(x,t)$

Gaussian of width $\sigma = \sqrt{2Dt}$



$\langle x\rangle$ – ? $\langle x^2\rangle$ – ?

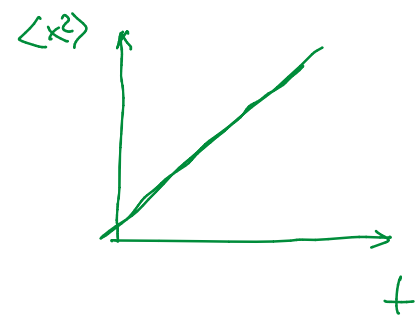
$$\langle x\rangle = \frac{\int x\, e^{-\frac{x^2}{4Dt}}\,dx}{\int e^{-\frac{x^2}{4Dt}}\,dx} = 0$$

even

Einstein diffusion equation

$$\langle x^2\rangle = 2\cdot\underbrace{\frac{\hbar^2}{2m}}_{D}\cdot t$$

coeff. of diffusion



Random walk algorithm:

- in a free space the solution of Laplace equation is a Gaussian
- $x_{i+1} = x_i + \xi_1 \cdot \Delta t$

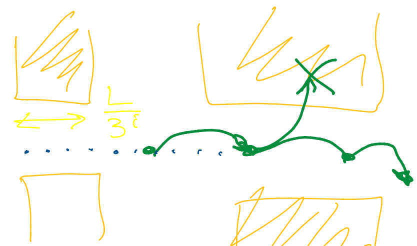
  $y_{i+1} = y_i + \xi_2 \cdot \Delta t$

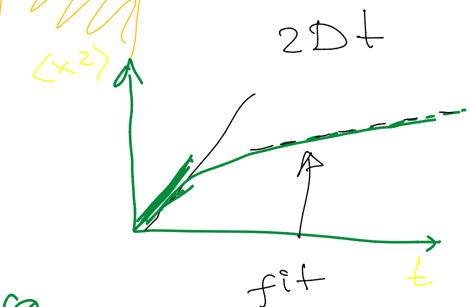
  with random values ξ_1, ξ_2 from a Gaussian distribution
- apply periodic boundary condition:

  if $x_{i+1} > L \rightarrow x_{i+1} := x_{i-1} - L$

  $x_{i+1} < 0 \rightarrow x_{i+1} := x_{i+1} + L$

- if (x_{i+1}, y_{i+1}) is in not-allowed region $\Rightarrow$ reject





$$\langle (x - x_0)^2 \rangle$$
$$\langle (y - y_0)^2 \rangle$$

$$\langle x^2 \rangle = 2D \cdot t$$
$$\langle y^2 \rangle = 2D \cdot t \quad , t \to 0$$

$$\langle x^2 \rangle = \text{const} + 2D' t , \quad t \to \infty$$

$$\frac{D'}{D} = \frac{D'}{\frac{\hbar^2}{2m}} - ?$$

Gaussian distribution Box Muller method

$0 < u_1 < 1$
$0 < u_2 < 1$ } 2 random values with uniform distributio

Polar coordinates (r, φ)

$$\varphi = 2\pi \cdot u_1 \quad ; \; 0 < \varphi < 2\pi$$

$$r = \sqrt{-2 \cdot \ln u_2}$$

$$\xi_1 = r \cdot \cos\varphi$$
$$\xi_2 = r \cdot \sin\varphi$$

Normal / Gaussian distribution

$$\exp\left(-\frac{x^2}{2}\right)$$

i.e. with width $\sigma = 1$

In our case $\sigma \to \Delta t$; $p = \exp\left(-\frac{1}{2}\frac{x^2}{\Delta t^2}\right)$

$$\begin{cases} x_{i+1} = x_i + \xi_1 \cdot \Delta t \\ y_{i+1} = y_i + \xi_2 \cdot \Delta t \end{cases}$$

$\Delta t \ll \frac{L}{3^i}$, i - iteracion

$\Delta t < \frac{1}{3} \cdot \frac{L}{3^i}$ should be sufficient

Tasks :

1) verify that in a free space

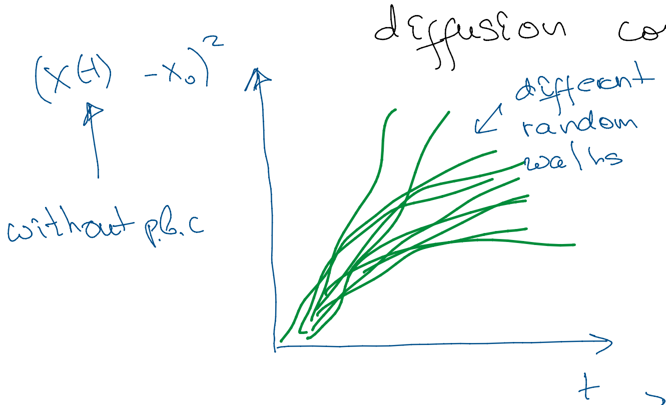
$$\langle x^2 \rangle = 2D \cdot t \quad , \quad D = \frac{\hbar^2}{2m}$$

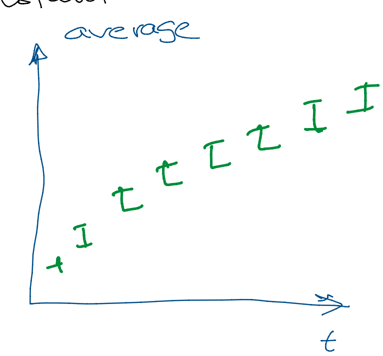
$$\langle x^2 \rangle = \frac{\hbar^2}{m} \cdot t$$

2) in the presence of the fractal

a) time evolution is diffusive?
$\langle x^2 \rangle$ linear in t ? $t \to \infty$

b) if yes, calculate the diffusion constant





calculate $\langle x^2 \rangle = \frac{1}{N_{RW}} \sum_{i=1}^{N_{RW}} (x_i - x_0)^2$

number of random walks