

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

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

$$f(x_i) = f_i, \quad i = 0, 1, \dots$$

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



p.b.c  $f'_0 = 0$

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

$$f'(x_0) = \frac{f_1 - f_{-1}}{2\Delta h} = 0$$

$$f_{-1} = f_1$$

z.b.c  $f_{-1} = 0$

$$\Delta \rightarrow$$

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

p.b.c  $f''_0 = \frac{f_1 - 2f_0 + f_{-1}}{2\Delta x^2} = \frac{2f_1 - 2f_0}{2\Delta x^2}$

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

$$\begin{pmatrix} f(x, y) = f(x) f(y) \\ \frac{\partial^2}{\partial x^2} \left( - \frac{\partial^2}{\partial x^2} \right) f(x) = E_x f(x) \\ \text{||-||} \qquad \qquad \qquad = E_y \end{pmatrix}$$

$$\begin{aligned}
 f(x,y) &= f(x) f(y) \\
 \frac{\hbar^2}{2m} \left( -\frac{\partial^2}{\partial x^2} \right) f(x) &= E_x f(x) \\
 \parallel - \parallel &= E_y \\
 \rightarrow &= E_x f(x) f(y) + E_y f(x) f(y) \\
 &= (E_x + E_y) f(x,y)
 \end{aligned}$$

$$E = E_x + E_y = 2E_x$$

g.g.

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

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

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

$$\begin{aligned}
 f''(x) &= -Ak^2 \sin kx - Bk^2 \cos kx \\
 &= -k^2 f(x)
 \end{aligned}$$

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

Free parameters  $A, B, k$

Boundary condition,

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

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

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

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

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

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

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

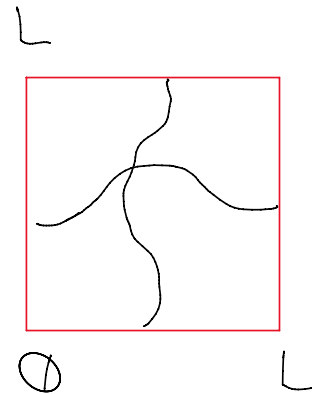
$$f\left(\frac{L}{2}\right) + f\left(-\frac{L}{2}\right) = 2B \cos \frac{kL}{2} = 0$$

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

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

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

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



$$\left\{ \begin{aligned} f(x,y) &= \sin \frac{\pi}{L} x \cdot \sin \frac{\pi}{L} y \end{aligned} \right.$$

$$f(x=0, y) = 0$$

$$f(x=L, y) = \sin \pi \cdot \dots = 0$$

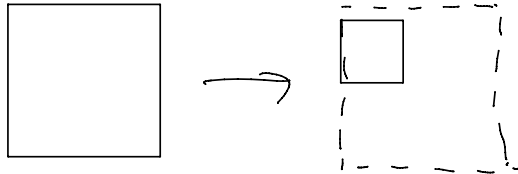
$$f(x,y) = \sin \frac{\pi}{L} \left(x - \frac{L}{2}\right) \cdot \cos \frac{\pi}{2} \left(x - \frac{L}{2}\right)$$

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

$$\psi(-\frac{L}{2}, y) = \sin \frac{\pi}{L}(-L) \dots = \sin(-\pi) = 0$$

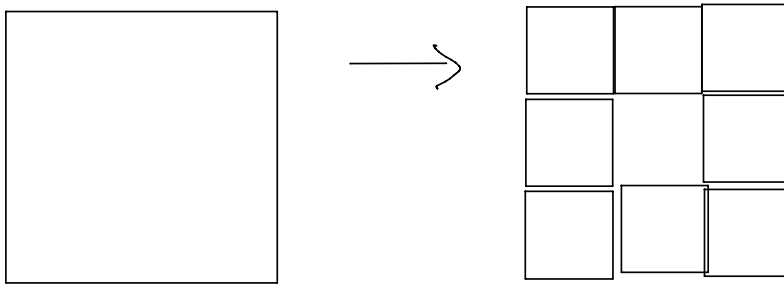
Energy upper bound:

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



$$E = \pi^2 \frac{\hbar^2}{mL^2} \rightarrow \pi^2 \frac{\hbar^2}{(L/3)^2 m} = \pi^2 g^1 \frac{\hbar^2}{mL^2}$$

2) Improved upper bound



iteration 1       $N$  squares       $N=8$

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

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

Iteration:

$$N_{\text{total}} = 9$$

$$N_{\text{occupied}} = 8$$

$$\tilde{N}_p = \frac{N_p}{N_{\text{total}}}$$

$$N_p = \sum_{\text{occupied}} \tilde{N}_p$$

$$= N_{\text{occupied}} \cdot \tilde{N}_p$$

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

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

$$\begin{aligned} E &= N_{\text{occupied}} \cdot \pi^2 \cdot \frac{\hbar^2}{m} \frac{N_p \cdot g^i}{N_{\text{occupied}} \cdot L^2} \\ &= \pi^2 g^i \frac{\hbar^2}{m L^2} \end{aligned}$$