Q1: Particle in a box

* L=10 atomik unit
* Delta function centered at x=5 atomic units
* in natural units, $\hbar$ and m are equal to 1

Trial wavefunction $\Phi(x) = \sum_{i=1}^{N} c_i \cdot \psi_i(x)$ $\quad \psi_n(x) = \sqrt{\frac{2}{10}} \cdot \sin\left(\frac{n \cdot \pi \cdot x}{10}\right)$

$$E[\Phi(x)] = \frac{\int_0^{\infty} \Phi^*(x) \cdot \hat{H} \cdot \Phi(x) \cdot dx}{\int_0^{\infty} \Phi^*(x) \cdot \Phi(x) \cdot dx}$$

Hamiltonian Operator: $-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \delta(x-5)$

$$E[\Phi(x)] \cdot \sum_{i=1}^{N} \sum_{j=1}^{N} c_i \cdot c_j \cdot S_{ij} = \sum_{i=1}^{N} \sum_{j=1}^{N} c_i \cdot c_j \cdot H_{ij}$$

$$S_{ij} = \int_0^L \psi_i(x) \cdot \psi_j(x) \cdot dx = \delta_{ij} \qquad H_{ij} = \int_0^L \psi_i(x) \cdot \hat{H} \cdot \psi_j(x) \cdot dx$$

$$H_{ij} = \int_0^L \sqrt{\frac{2}{10}} \cdot \sin\left(\frac{i \cdot \pi \cdot x}{10}\right) \hat{H} \cdot \sqrt{\frac{2}{10}} \cdot \sin\left(\frac{j \cdot \pi \cdot x}{10}\right) \cdot dx$$

Hamiltonian operator acting on $\psi_j(x)$

$$H_{ij} = \int_0^L \sqrt{\frac{2}{10}} \cdot \sin\left(\frac{i \cdot \pi \cdot x}{10}\right) \cdot \left[\left(-\frac{\hbar^2}{2m} \cdot \frac{d^2}{dx^2} + \delta(x-5)\right) \sqrt{\frac{2}{10}} \sin\left(\frac{j \cdot \pi \cdot x}{10}\right)\right] dx$$

$$H_{ij} = \int_0^L \sqrt{\frac{2}{10}} \cdot \sin\left(\frac{i \cdot \pi \cdot x}{10}\right) \left[\left(\frac{\hbar^2 \cdot \pi^2 \cdot n^2}{2mL^2} + \delta(x-5)\right)\right) \sqrt{\frac{2}{10}} \cdot \sin\left(\frac{j \cdot \pi \cdot x}{10}\right) dx$$

$n^2 \rightarrow j^2$

$$H_{ij} = \int_0^L \sqrt{\frac{2}{10}} \cdot \sin\left(\frac{i \cdot \pi \cdot x}{10}\right) \cdot \frac{\hbar^2 \pi^2 j^2}{2mL^2} \cdot \sqrt{\frac{2}{10}} \sin\left(\frac{j \cdot \pi \cdot x}{10}\right) dx +$$

$$\boxed{\int_0^L \sqrt{\frac{2}{10}} \cdot \sin\left(\frac{i \cdot \pi \cdot x}{10}\right) \cdot \delta(x-5) \cdot \sqrt{\frac{2}{10}} \sin\left(\frac{j \cdot \pi \cdot x}{10}\right) dx} \rightarrow A$$

$$A = \sqrt{\frac{2}{10}} \cdot \sin\left(\frac{n \cdot \pi \cdot 5}{\cancel{10}\,2}\right) * \sqrt{\frac{2}{10}} \cdot \sin\left(\frac{n \cdot \pi \cdot 5}{\cancel{10}\,2}\right)$$

$$\boxed{\frac{L}{2} = \int_0^L \sin\left(\frac{n \cdot \pi \cdot x}{L}\right) \cdot \sin\left(\frac{n \cdot \pi \cdot x}{L}\right) dx}$$

If $i=j$ $\delta_{ij}=1$ for particle in a box
$i \neq j$ $\delta_{ij}=0$ normalization
$i=j$ Integral = 1

$$H_{ij} = \frac{\cancel{2}}{10} \cdot \frac{10}{2} \frac{\hbar^2 \pi^2 j^2}{2mL^2} \int_0^{10} \sin\left(\frac{i \cdot \pi \cdot 5}{10}\right) \cdot \sin\left(\frac{j \cdot \pi \cdot 5}{10}\right) dx + \rightarrow \delta_{ij}$$

If $i=j$ $\delta_{ij}=1$
If $i \neq j$ $\delta_{ij}=0$

$$\frac{\cancel{2}}{\cancel{10}\,5} \cdot \sin\left(\frac{i \cdot \pi}{2}\right) \cdot \sin\left(\frac{j \cdot \pi}{2}\right)$$

$$H_{ij} = \frac{j^2 \cdot \pi^2}{200} \int_0^{10} \sin\left(\frac{i \pi}{2}\right) \cdot \sin\left(\frac{j \pi}{2}\right) + \frac{1}{5} \sin\left(\frac{i \cdot \pi}{2}\right) \cdot \sin\left(\frac{j \cdot \pi}{2}\right)$$