Matrix Mechanics

We previously stated that using expansion theorem:

$$\psi(x) = \sum_i a_i \psi_i(x)$$

Suppose we apply an operator to this:

$$\hat{O}\psi(x) = \sum_i a_i \hat{O}\psi_i(x)$$

The effect of an operator on any eigenfunction will produce a wave function that can be represented as a sum of the original eigenfunctions. So:

$$\hat{O}\psi_i(x) = \sum_j O_{ji}\psi_j(x)$$

substituting this into our previous expression:

$$\hat{O}\psi(x) = \sum_i a_i \hat{O}\psi_i(x) = \sum_{ij} O_{ji} a_i \psi_j(x)$$

We can find O_{ji} coefficients using orthonormality:

$$\langle \psi_k | \hat{O} | \psi_i \rangle = \sum_j O_{ji} \langle \psi_k | \psi_j \rangle = \sum_j O_{ji} \delta_{jk} = \underline{O_{ki}}$$

This is one element of the matrix.

Let's do an example.

Consider an infinite square well of width $2a$ from $x = 0$ to $x = 2a$. From Quantum physics last year, we know

$$E_n = \frac{\hbar^2 \pi^2 n^2}{8ma^2}$$

where n is a positive integer. These are the eigenvalues

The associated eigenfunctions are

$$\psi_n(x) = \frac{1}{\sqrt{a}} \sin\left(\frac{n\pi x}{2a}\right)$$

We can represent the eigenvalues in matrix form:

$$\frac{\hbar^2 \pi^2}{8 M a^2} \begin{bmatrix} 1 & 0 & 0 & \cdots \\ 0 & 4 & 0 & \\ 0 & 0 & 9 & \\ \vdots & & & \end{bmatrix}$$

so we can write $\hat{H}\psi = E\psi$ with each term being a matrix.