

# Finite difference Operator derivation 1

$$\hat{\pi} = -i \frac{d}{d\theta} \quad \hat{\pi}^2 = -\frac{d^2}{d\theta^2}$$

$$\hat{\pi} = \begin{pmatrix} -i \frac{\partial}{\partial \theta} & 0 \\ 0 & i \frac{\partial}{\partial \theta} \end{pmatrix} \quad \hat{\pi}^2 = -\frac{\partial^2}{\partial \theta^2}$$

Need to replace this with an <sup>matrix</sup> operator  
first need to get expression of  
2<sup>nd</sup> order derivative: Taylor expand

$$\psi(\theta + \delta\theta) \quad \text{and} \quad \psi(\theta - \delta\theta)$$

$$\psi(\theta - \delta\theta) = \psi(\theta) - \delta\theta \psi'(\theta) + \frac{\delta\theta^2}{2!} \psi''(\theta) - \frac{\delta\theta^3}{3!} \psi'''(\theta)$$

$$\psi(\theta + \delta\theta) = \psi(\theta) + \delta\theta \psi'(\theta) + \frac{\delta\theta^2}{2!} \psi''(\theta) + \frac{\delta\theta^3}{3!} \psi'''(\theta)$$

$$\psi(\theta - \delta\theta) + \psi(\theta + \delta\theta) = 2\psi(\theta) + \delta\theta^2 \psi''(\theta) + O(\delta\theta^2)$$

$$\psi''(\theta) = \frac{\psi(\theta - \delta\theta) + \psi(\theta + \delta\theta) - 2\psi(\theta)}{\delta\theta^2}$$

$$\psi''(\theta_n) = (\psi(\theta_{n-1}) + \psi(\theta_{n+1}) - 2\psi(\theta_n)) / \delta\theta^2$$

$$\therefore \langle \psi_n | \pi^2 | \psi_m \rangle = \langle \psi_n | -\psi_{n-1} - \psi_{n+1} + 2\psi_n \rangle = M_{nm}$$

$$= \langle \psi_n | -\psi_{n-1} - \psi_{n+1} + 2\psi_n \rangle = M_{nm}$$

$$\text{for } n = m-1 \Rightarrow M_{nm} = -1$$

$$n = m+1 \Rightarrow M_{nm} = -1$$

$$n = m \Rightarrow M_{nm} = 2$$

$$n \neq m, m+1, m-1 \Rightarrow M_{nm} = 0$$

$$\therefore \langle \Psi | \pi^2 | \Psi \rangle = \frac{1}{8\theta^2} \begin{pmatrix} 2 & -1 & 0 & 0 & \dots & -1 \\ -1 & 2 & -1 & 0 & 0 & \dots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \dots & -1 & 2 & -1 \\ -1 & 0 & 0 & \dots & -1 & 2 \end{pmatrix}$$

$$(N_1 - Q_1) \Psi = (Q_1 - Q_2) \Psi$$

$$(Q_1 - Q_2) \Psi = (Q_2 - Q_3) \Psi = \dots = (Q_{n-1} - Q_n) \Psi$$

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