COMPUTATIONAL QUANTUM PHYSICS

Quantum Mechanics in 1 Hour

State of a system is described by $|\psi\rangle \in \mathcal{H}$

$\| \, |\psi\rangle \, \| = 1 \quad \rightsquigarrow$ Normalized

$\langle \phi | \psi \rangle \quad \rightsquigarrow$ Inner Product Btw Vectors

$\langle \psi | \psi \rangle = 1 \quad \rightsquigarrow$ Normalization

Example: Spin 1/2

$$|\psi\rangle \in \mathbb{C}^2$$

$$|\psi\rangle = \alpha \, | S_z ; + \rangle + \beta \, | S_z ; - \rangle$$

$$= \alpha |\uparrow\rangle + \beta |\downarrow\rangle$$

$$\left.\begin{array}{l} \text{Prob}(\uparrow) = |\alpha|^2 \\ \text{Prob}(\downarrow) = |\beta|^2 \end{array}\right\} \text{Measurement Postulate}$$

$$\text{Prob}(\uparrow) + \text{Prob}(\downarrow) = |\alpha|^2 + |\beta|^2 = 1$$

$$|\rightarrow\rangle = |S_x ; +\rangle = \frac{1}{\sqrt{2}}\left[\,|\uparrow\rangle + |\downarrow\rangle\,\right]$$

$$|\leftarrow\rangle = |S_x ; -\rangle = \frac{1}{\sqrt{2}}\left[\,|\uparrow\rangle - |\downarrow\rangle\,\right]$$

examples of eigenstates of S_x

Mixed States and Density Matrices

$$\hat{\rho} = \sum_i P_i \, |\psi_i\rangle\langle\psi_i|$$

P_i: Probability of having a pure state $|\psi_i\rangle$

$$\mathrm{Tr}\,\hat{\rho} = \mathbb{1} \quad \rightarrow \text{Normalization Condition}$$

$$\mathrm{Tr}\,\hat{\rho} = \sum_x \langle x|\hat{\rho}|x\rangle = \sum_x \sum_i \langle x|\psi_i\rangle\langle\psi_i|x\rangle P_i$$

$$\mathrm{Tr}\,\hat{\rho} = \sum_i \underbrace{\sum_x |\langle x|\psi_i\rangle|^2}_{1} P_i = \sum_i P_i = 1$$

Recover Pure States:

$$\hat{\rho}_{PURE} \rightsquigarrow |\psi_e\rangle, \quad P_i = \delta_{ie}$$

$$\hat{\rho}_{PURE} = |\psi_e\rangle\langle\psi_e|$$

Example:

$$\langle\uparrow|\hat\rho_{\rightarrow}|\uparrow\rangle = \langle\uparrow|\rightarrow\rangle\langle\rightarrow|\uparrow\rangle = 1/2$$

$$\hat\rho_{\rightarrow} = |\rightarrow\rangle\langle\rightarrow| = \begin{pmatrix} 1/2 & 1/2 \\ 1/2 & 1/2 \end{pmatrix}$$

off Diagonal ?

Ex: $\hat\rho_{MIXED}$ $\sim$ 50% having $|\uparrow\rangle$, $\sim$ 50% having $|\downarrow\rangle$ $\Big\} = \frac{1}{2}|\uparrow\rangle\langle\uparrow| + \frac{1}{2}|\downarrow\rangle\langle\downarrow|$

$$\hat\rho_{MIXED} = \begin{pmatrix} 1/2 & 0 \\ 0 & 1/2 \end{pmatrix}$$

OBSERVABLES $\rightsquigarrow$ HERMITIAN OPERATORS

$$\hat S_x = \frac{\hbar}{2}\hat\sigma_x = \begin{pmatrix} 0 & \hbar/2 \\ \hbar/2 & 0 \end{pmatrix}$$

$$\hat S_y = \frac{\hbar}{2}\hat\sigma_y = \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

$$\hat S_z = \frac{\hbar}{2}\hat\sigma_z = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$[\hat S_x, \hat S_y] = i\hbar \hat S_z$$

$$[\hat S_\alpha, \hat S_\beta] = i\hbar\, \varepsilon_{\alpha\beta\gamma} \hat S_\gamma$$

Levi-Civita Symbol

THE MEASUREMENT PROCESS

$$|\psi\rangle \xrightarrow[\text{Collapse}]{\hat{A}} |A_i\rangle \quad \text{Eigenstate}$$

$$a_i \quad \text{eigenvalue}$$

$$\hat{A}\,|A_i\rangle = a_i\,|A_i\rangle$$

Example: $|\psi\rangle = |\uparrow\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$

$$\hat{\rho}_\uparrow = |\uparrow\rangle\langle\uparrow| = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$$

<u>Measure S_x</u>

After the measurement $|\psi\rangle$

$$|\rightarrow\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

$$|\leftarrow\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix}$$

$$P_\rightarrow = \| \langle\rightarrow|\psi\rangle \|^2 = \frac{1}{2}$$

$$P_\leftarrow = \| \langle\leftarrow|\psi\rangle \|^2 = \frac{1}{2}$$

$$\hat{\rho} = P_\rightarrow |\rightarrow\rangle\langle\rightarrow| + P_\leftarrow |\leftarrow\rangle\langle\leftarrow|$$

$$\hat{\rho} = \begin{pmatrix} 1/2 & 0 \\ 0 & 1/2 \end{pmatrix}$$

Expectation Values:

$$\langle A \rangle = \langle \psi | \hat{A} | \psi \rangle$$ ⇝ Mean Value

$$\langle A \rangle = \mathrm{Tr}(\hat{\rho} \hat{A})$$

If $\hat{\rho}_\psi = |\psi\rangle\langle\psi|$

$$\langle A \rangle = \mathrm{Tr}(\hat{\rho} \hat{A}) = \sum_x \langle x | \psi \rangle \langle \psi | \hat{A} | x \rangle$$

$$= \sum_x \langle \psi | \hat{A} | x \rangle \langle x | \psi \rangle = \langle \psi | \hat{A} | \psi \rangle$$

Schrödinger Equations

$$i\hbar \frac{\partial}{\partial t} |\psi(t)\rangle = \hat{H} |\psi(t)\rangle$$ → Time Dependent Sch. Equation

$$\hat{U}(t) = e^{-\frac{i\hat{H}t}{\hbar}}$$

$$\hat{H} |\psi_k\rangle = E_k |\psi_k\rangle$$ ⇝ Eigenvalue Problem (Time Independent)

NP HARD (?)

$$|\psi(t)\rangle = e^{-i\frac{\hat{H}t}{\hbar}} |\psi(0)\rangle$$

$$= \sum_k e^{-i\frac{\hat{H}t}{\hbar}} |\psi_k\rangle \underbrace{\langle\psi_k|\psi(0)\rangle}$$

$$|\psi(t)\rangle = \sum_k e^{-i\frac{E_k t}{\hbar}} |\psi_k\rangle C_k$$

Density Matrix Time Evolution

$$i\hbar \frac{\partial}{\partial t} \hat{\rho}(t) = [\hat{H}, \hat{\rho}(t)]$$

Thermal Density Matrix

$$\beta = \frac{1}{k_B T}, E_k \qquad p_k = \frac{1}{Z} e^{-\beta E_k}$$

$$Z = \sum_k \exp(-\beta E_k)$$

Quantum

$$|\psi_k\rangle, \quad E_k \qquad \hat{\rho}_\beta = \sum_k P_k |\psi_k\rangle\langle\psi_k|$$

$$= \frac{1}{Z} \sum_k e^{-\beta E_k} |\psi_k\rangle\langle\psi_k|$$

Computing Averages:

$$\langle A \rangle = \mathrm{Tr}(\hat{A}\,\hat{\rho}_B) = \frac{\mathrm{Tr}\ \hat{A}\exp(-\beta\hat{H})}{\mathrm{Tr}\exp(-\beta\hat{H})}$$

$$\mathrm{Tr}\ e^{-\beta\hat{H}} = \sum_k \langle \psi_k | e^{-\beta\hat{H}} | \psi_k \rangle = \sum_k e^{-\beta E_k} = Z$$

Particles in free space

n- Dimensional Space

$\hat{\vec{X}} \rightsquigarrow$ position operator

$\hat{\vec{p}} \rightsquigarrow$ momentum operator

$$\langle \vec{x} | \psi \rangle = \psi(\vec{x}) \in \mathbb{C}^n$$

↳ Wave Function Particles

$$\hat{p}_\alpha = -i\hbar \widehat{\frac{\partial}{\partial x_\alpha}}$$

$$[\hat{x}_\alpha, \hat{p}_\beta] = i\hbar\,\delta_{\alpha\beta}$$

Hamiltonian

$$H(\vec{x}, \vec{p}) = \frac{|\vec{p}|^2}{2m} + V(\vec{x})$$

Classical Hamiltonian

$$\hat{H} = \frac{|\hat{\vec{p}}|^2}{2m} + V(\vec{x})$$

$$= \frac{-\hbar^2}{2m} \sum_{\alpha=1}^{m} \frac{\partial^2}{\partial x_\alpha^2} + V(\vec{x})$$

$$= \frac{-\hbar^2}{2m} \vec{\nabla}^2 + V(\vec{x})$$

Time Dependent Schrödinger Equation:

$$i\hbar \frac{\partial}{\partial t} \langle \vec{x} | \psi \rangle = \langle \vec{x} | \hat{H} | \psi(t) \rangle$$

$$i\hbar \frac{\partial}{\partial t} \psi(x,t) = -\frac{\hbar^2}{2m} \nabla^2 \psi(\vec{x},t) + V(\vec{x}) \psi(\vec{x},t)$$