

## Basics of QM

### Classical Recap

$$H = \frac{p^2}{2m} + V(q); \quad \dot{q} = \frac{\partial H}{\partial p}; \quad \dot{p} = -\frac{\partial H}{\partial q} = -\frac{\partial V}{\partial q}$$

### Quantum Mechanics

$$H_{op} = \frac{p_{op}^2}{2m} + V(q); \quad p_{op} = -i\hbar \frac{\partial}{\partial q} \quad \text{- one degree of freedom}$$

$$H_{op} = -\frac{\hbar^2}{2m} \nabla^2 + V(\mathbf{q}); \quad p_{op} = -i\hbar \nabla = -i\hbar \left( \frac{\partial}{\partial x} \hat{x} + \frac{\partial}{\partial y} \hat{y} + \frac{\partial}{\partial z} \hat{z} \right) \quad \text{- 3dof}$$

### The Schrödinger equation(s)

$$i\hbar \frac{\partial}{\partial t} \psi = H_{op} \psi \quad \text{- Most general, time dependent}$$

$$\psi(\mathbf{q}, t) = e^{-iH_{op}t/\hbar} \psi(\mathbf{q}, 0) = (1 - H_{op}t/\hbar + \dots) \psi(\mathbf{q}, 0) \quad \text{- Formal solution for time independent Hamiltonians}$$

For special class of wavefunctions, which are termed the eigenfunctions

$$H_{op} \psi_n = E_n \psi_n \quad \text{- Time independent}$$

This set of functions have the following properties:

$$\int \psi_n^* \psi_m = \delta_{n,m} = 1 \text{ if } m = n, \quad 0 \text{ if } m \neq n \quad \text{- orthonormal}$$

Dirac invented notation for this integral:  $\langle n | m \rangle = \delta_{n,m}$

Then a special solution to the time-dependent Schrödinger equation is

$$\psi_n(t) = e^{-iE_n t / \hbar} \psi_n$$

The general solution is

$$\psi(t) = \sum_n C_n e^{-iE_n t / \hbar} \psi_n, \text{ where the expansion coefficients are given by}$$

$$C_n = \langle n | \psi(0) \rangle$$

### Matrix elements and Expectation values:

$$A_{m,n} = \langle m | A_{op} | n \rangle = \int \psi_m^* A_{op} \psi_n$$

$$= \langle A_{op} | m \rangle = \int \psi_m^* A_{op} \psi_n$$

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Hermitian operator  $A_{op}$ :

$$\text{But } \langle A_{op} | m \rangle = \langle n | A_{op} | m \rangle^*, \text{ so}$$

$$A_{m,n} = (A_{n,m})^*$$