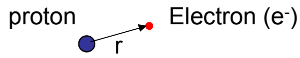
Part 1: bonding

- Why we need Quantum Mechanics?
  - The hydrogen atom
- Basic Quantum Mechanics
  - Schrodinger equation and simple solutions
- Electronic structure of atoms
  - Hydrogen and multi-electron atoms
- Bonding in molecules
  - The simplest molecule H2+
  - First row hydrides
  - Covalent, ionic and van der Waals interactions
- Bonding in crystalline solids
  - Band structure
  - Covalent vs. metallic bonding

Part 2: Symmetry, crystal structure and crystallography

- Relationship between bonding and crystal structure
- Lattices Planes and Directions
- Symmetry in 2D & 3D
- Building crystal structures in 3D
- Defects

The simplest atom: hydrogen



What if we treat it with classical mechanics?

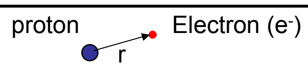
Energy: $$E = -\frac{e^2}{|r|} + \frac{|p|^2}{2m}$$

State with minimum energy (equilibrium)?

r=0

- The Hydrogen atom collapses to zero size
- No atoms, no molecules …

The hydrogen atom



Quantum mechanics

Wave function: a function of position (r) that describes the probability of finding the electron at position r

$$\psi(\vec{r})$$

전자가 발견될 확률

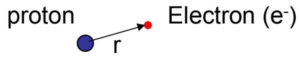
Physical Observable → operator

Position: multiply the WF by r $\vec{r}$

Momentum: involves the gradient of the WF $$\vec{p} = \frac{\hbar}{i}\vec{\nabla} = \frac{\hbar}{i}\left(\frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z}\right)$$

Energy:
(Hamiltonian) $$E = -\frac{q^2}{|r|} - \frac{\hbar^2}{2m}\vec{\nabla}\cdot\vec{\nabla} = -\frac{q^2}{|r|} - \frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right)$$

The hydrogen atom



Quantum mechanics

If you perform an experimental measurement what you obtain is the expectation value of the associated operator:

Definition of "expectation value":

$$\langle O \rangle = \int \psi(\vec{r}) O \psi(\vec{r}) dxdydz$$

Integral over all space

Example: average position

$$\langle \vec{r} \rangle = \int \psi(\vec{r}) \vec{r} \psi(\vec{r}) dxdydz = \int \vec{r} \psi(\vec{r})^2 d^3 r$$

›babilities

ɜs and calculate the average number you get

Back to expectation values:

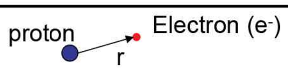
Average position

$$\langle \vec{r} \rangle = \int \psi(\vec{r})\vec{r}\,\psi(\vec{r})dxdydz = \int \vec{r}\,\psi(\vec{r})^2 d^3 r$$

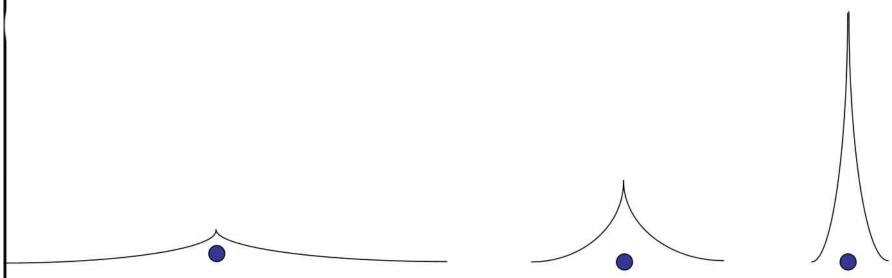
Average momentum

$$\langle \vec{p} \rangle = \int \psi(\vec{r})\left[\frac{\hbar}{i}\left(\frac{\partial}{\partial x},\frac{\partial}{\partial y},\frac{\partial}{\partial z}\right)\right]\psi(\vec{r})dxdydz =$$

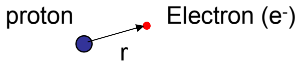
The hydrogen atom



$$\langle H \rangle = \int d^3 r \Psi^*(r)\left[-\frac{\hbar\nabla^2}{2m}-\frac{e^2}{r}\right]\Psi(r)$$



Summary



Classical mechanics

State of the system:

$\vec{r}(t) \quad \vec{p}(t)$

Energy:

$$V = \frac{q_i q_j}{r} = -\frac{e^2}{r}$$

$$K = \frac{p^2}{2m} = \frac{1}{2}mv^2$$

Ground state (minimum energy):

$$r = 0$$

$$E = -\infty$$

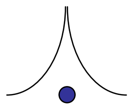
Atoms do not exist!!

Classical mechanics fails: quantum mechanics

State: wave function: $\psi(\vec{r})$

Energy: $E = -\frac{\hbar^2}{2m}\nabla^2 - \frac{e^2}{r}$

Ground state: finite size



The Kinetic energy make atoms stable