Schrödinger equation for the hydrogen atom:

reduced Planck's constant

For H nucleus Z = 1.

Laplace operator $\left(\frac{d^2}{dr^2}\right)$

elementary charge.

$$\left(\frac{-\hbar^2}{2m_e}\nabla^2 - \frac{1e^2}{4\pi\varepsilon_0|\vec{r}-\vec{R}|}\right)\Psi_e(\vec{r}) = E_e\Psi_e(\vec{r})$$

mass of an electron

distance.

dielectric in vacuum

Removing constants, and considering atomic units: $m_e = \hbar = e = 4\pi\varepsilon_0 = 1$

this results in the unit *Hartree*

Eigenfunctions of the **hydrogen atom** are called **atomic orbitals**.

Component	Depends on	concerns
Radial	n	Distance from nucleus (r)
Angular	m_l , l	Angle from nucleus

Orbital: a one-electron wave function in three dimensional space.

MO Theory: **The Hartree Product:**

Separation of variables to a multielectron wave function results in the hartree product; the multiplication of the molecular orbitals.

e.g. For a 2-electron system: $\Psi_e(1,2) \approx \phi_1(1)\phi_2(2) \pm \phi_2(1)\phi_1(2)$

± + bosonic WF
− fermonic WF

Electrons are indistinguishable particles, and we can't really assign them numbers like '1' or '2'. Therefore, we have to account for the number of permutations.

They're also fermionic; so we consider only the 'negative' of permuted functions.

$$\Psi(1,2) = \phi_1(1)\phi_2(2) - \phi_2(1)\phi_1(2)$$

$$\Psi(2,1) = \phi_1(2)\phi_2(1) - \phi_2(2)\phi_1(1) = \boxed{-\Psi(1,2)}$$

Fermionic character

Boson	Particle with integer spin (photon, deuterium nucleus)
Fermion	Particle with half integer spin (electron, ^{13}C nucleus)