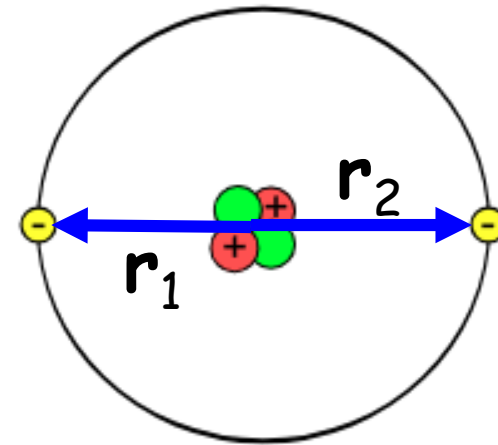


Chapter 5: Identical Particles

For **one particle**, like one electron in the H atom, we simply need the wave function $\Psi(\mathbf{r}_1, t)$ where \mathbf{r}_1 is the coordinate of electron "1".

Consider now **two particles**.

For **two particles**, e.g. two electrons in the He atom, in QM we need the wave function $\Psi(\mathbf{r}_1, \mathbf{r}_2, t)$ where \mathbf{r}_1 and \mathbf{r}_2 are the coordinates of the two electrons.

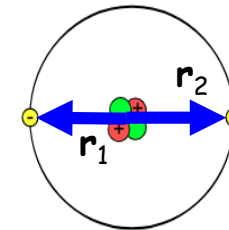


Mathematically, the Sch. Eq. $i\hbar \frac{\partial \Psi}{\partial t} = H\Psi$ has a more complicated Hamiltonian.

$$H = -\frac{\hbar^2}{2m_1} \nabla_1^2 - \frac{\hbar^2}{2m_2} \nabla_2^2 + V(\mathbf{r}_1, \mathbf{r}_2, t)$$

The potential V typically includes e-proton attraction, but also **e-e repulsion**.

Example, for the He atom:



$$H = \left\{ -\frac{\hbar^2}{2m} \nabla_1^2 - \underbrace{\frac{1}{4\pi\epsilon_0} \frac{2e^2}{r_1}}_{\substack{\text{p-e}_1 \text{ attraction} \\ \text{is called } V(\mathbf{r}_1)}} \right\} + \left\{ -\frac{\hbar^2}{2m} \nabla_2^2 - \underbrace{\frac{1}{4\pi\epsilon_0} \frac{2e^2}{r_2}}_{\substack{\text{p-e}_2 \text{ attraction} \\ \text{is } V(\mathbf{r}_2)}} \right\} + \underbrace{\frac{1}{4\pi\epsilon_0} \frac{e^2}{|\mathbf{r}_1 - \mathbf{r}_2|}}_{\substack{\text{e}_1\text{-e}_2 \text{ repulsion} \\ \text{is } V(\mathbf{r}_1, \mathbf{r}_2)}}$$

If the particles do not interact with one another, *e.g. if we drop the e-e repulsion*, we call them "noninteracting".

In this case, $V(\mathbf{r}_1, \mathbf{r}_2, t) = V(\mathbf{r}_1, t) + V(\mathbf{r}_2, t) + \cancel{V(\mathbf{r}_1, \mathbf{r}_2)}$.

Example: two particles inside a capacitor, far from each other. Then, it is a good approx. that each electron is just immersed in the potential V of the capacitor.

Amazingly, "noninteracting", a CRUDE approx., is sometimes a GOOD approx. *qualitatively even in atoms.*

For non-interacting particles a wave function solution of the Sch. Eq. is just the product $\Psi(\mathbf{r}_1, \mathbf{r}_2, t) = \Psi_a(\mathbf{r}_1, t)\Psi_b(\mathbf{r}_2, t)$ where a and b are quantum numbers, such as those of the H atom (n, l, m_l) or the square well. Check!

E.g., in the H atom we could have,

$$\Psi(\mathbf{r}_1, \mathbf{r}_2, t) = \Psi_{100}(\mathbf{r}_1, t) \Psi_{21-1}(\mathbf{r}_2, t).$$

Its energy is $E = E_{100} + E_{21-1}$ (using $-2e^2$ as charge!)

Another eigenstate: $\Psi(\mathbf{r}_1, \mathbf{r}_2, t) = \Psi_{530}(\mathbf{r}_1, t) \Psi_{321}(\mathbf{r}_2, t).$

Its energy is $E = E_{530} + E_{321}$. Please check!

NOTE: Linear combinations can be made. E.g. consider

$$\Psi(\mathbf{r}_1, \mathbf{r}_2, t) = (3/5) \Psi_{100}(\mathbf{r}_1, t) \Psi_{21-1}(\mathbf{r}_2, t) + (4/5) \Psi_{530}(\mathbf{r}_1, t) \Psi_{321}(\mathbf{r}_2, t).$$

Normalized to one already. Quantum superposition !

But now the electrons are "quantum entangled" because if by measuring we find particle 1 is in 100, then particle 2 must be in 21-1. The electrons instantly know about what is happening to the other one. We can repeat the same discussion as last lecture for spins.

So far, all was for **noninteracting** electrons.

The e-e repulsion, makes everything far more “**complicated**” because it “**correlates**” the electrons: if one electrons is say on the left, by mere repulsion the other tends to be on the right. There is an entire field of ongoing research called “**strongly correlated electrons**”.

Here, wave functions are not just linear combinations of products of H atom wavefunctions. We will return to this ...

Finally, as usual, in all cases we must **normalize** to 1 because of the probabilistic interpretation:

$$\int |\Psi(\mathbf{r}_1, \mathbf{r}_2, t)|^2 d^3\mathbf{r}_1 d^3\mathbf{r}_2 = 1$$

5.1.1 Bosons and Fermions

First, for **simplicity**, let us **neglect the e-e repulsion**.
The energy levels are the **same** as in the H atom.

Assume one particle is in state "a" (e.g. 1s, spin up) and the other particle is in state "b" (e.g. 2s, spin down).

Then, in this particular case **IF e-e is neglected**, the wave function is the product:

$$\psi(\mathbf{r}_1, \mathbf{r}_2) = \psi_a(\mathbf{r}_1)\psi_b(\mathbf{r}_2)$$

As already explained, to prove this, use as potential V simply the sum of two H-atom terms, one per particle i.e. just the $p-e_1$ and $p-e_2$ attractions.

However, the key new concept is that if electrons are **identical**, then we **cannot** say "electron 1 is in $(1s, \uparrow)$ ". We can only say "**an electron is in $(1s, \uparrow)$** ".

In **classical physics** we can always "follow" particles and tell them apart, even if identical.
READ discussion in book page 201.

In **quantum physics** we **cannot** follow particles.
We only know probabilities.

Thus, if one electron is in state "a" and one electron in state "b", we must **symmetrize** the wave function to account for particles being identical.

One way to symmetrize is to **add** the two cases:

$$\psi_{+}(\mathbf{r}_1, \mathbf{r}_2) = A[\psi_a(\mathbf{r}_1)\psi_b(\mathbf{r}_2) + \psi_b(\mathbf{r}_1)\psi_a(\mathbf{r}_2)]$$

In what sense this has been "symmetrized"?

When \mathbf{r}_1 and \mathbf{r}_2 are exchanged, the first term becomes the second, and the second the first.

Then:

$$\psi_{+}(\mathbf{r}_1, \mathbf{r}_2) = \psi_{+}(\mathbf{r}_2, \mathbf{r}_1)$$

This case "+" applies to elementary particles called **bosons**.

Because in QM we only care about the wave function in absolute value, there is **another** possible combination !

$$\psi_{-}(\mathbf{r}_1, \mathbf{r}_2) = A[\psi_a(\mathbf{r}_1)\psi_b(\mathbf{r}_2) - \psi_b(\mathbf{r}_1)\psi_a(\mathbf{r}_2)]$$

In this case, when \mathbf{r}_1 and \mathbf{r}_2 are exchanged, we collect a minus sign in front:

$$\psi_{-}(\mathbf{r}_1, \mathbf{r}_2) = -\psi_{-}(\mathbf{r}_2, \mathbf{r}_1)$$

Elementary particles where the "-" applies are called **fermions**.

In summary, we have to accept as **another law of Nature** that elementary particles are either **bosons**, for the + case, or **fermions**, for the - case.

Moreover, there is a link between the sign +- in the combination and the value of the spin. **This can be shown within relativistic QM.**

bosons \leftrightarrow integer spin (examples: photon, phonon)

fermions \leftrightarrow half-integer spin (example: electron).

If two electrons are in the same state, such as $(1s, \uparrow)$, i.e. **including spin**, then the "-" wave function cancels:

$$\psi_{-}(\mathbf{r}_1, \mathbf{r}_2) = A[\psi_a(\mathbf{r}_1)\psi_a(\mathbf{r}_2) - \psi_a(\mathbf{r}_1)\psi_a(\mathbf{r}_2)] = 0$$

Then, the famous **Pauli principle** can be **deduced** from the fact that electrons are fermions.

This is somewhat similar to the case when we **deduced** the **uncertainty principle** in QM411.

It is important to keep the number of arbitrary laws to a minimum!

Let us define the exchange operator \hat{P} .

$$\hat{P} \psi(\mathbf{r}_1, \mathbf{r}_2) = \psi(\mathbf{r}_2, \mathbf{r}_1)$$

Applying \hat{P} twice:

$$\hat{P} \hat{P} \psi(\mathbf{r}_1, \mathbf{r}_2) = \hat{P} \psi(\mathbf{r}_2, \mathbf{r}_1) = \psi(\mathbf{r}_1, \mathbf{r}_2)$$

Because $\hat{P}^2 = 1$ as operator, then the eigenvalues are +1 and -1. **Check!**

Also $[\hat{H}, \hat{P}] = 0$:

$$\hat{H} = \left\{ -\frac{\hbar^2}{2m} \nabla_1^2 - \frac{1}{4\pi\epsilon_0} \frac{2e^2}{r_1} \right\} + \left\{ -\frac{\hbar^2}{2m} \nabla_2^2 - \frac{1}{4\pi\epsilon_0} \frac{2e^2}{r_2} \right\} + \frac{1}{4\pi\epsilon_0} \frac{e^2}{|\mathbf{r}_1 - \mathbf{r}_2|}$$
