Exchange Symmetry

We will first review of the quantum mechanics of multi-particle systems.

This will be vitally important for understanding many aspects of particle physics. (e.g. the quark model)

In particular: exchange symmetry.

In a multi-particle system, the wave function for the whole system is $\psi(\vec{r}_1, \vec{r}_2, \ldots)$ where $\vec{r}_i$ is the coordinate of particle i.

We will simplify our discussion to a 2 particle system.

Two Particle Systems

What if the two particles in the system are identical?

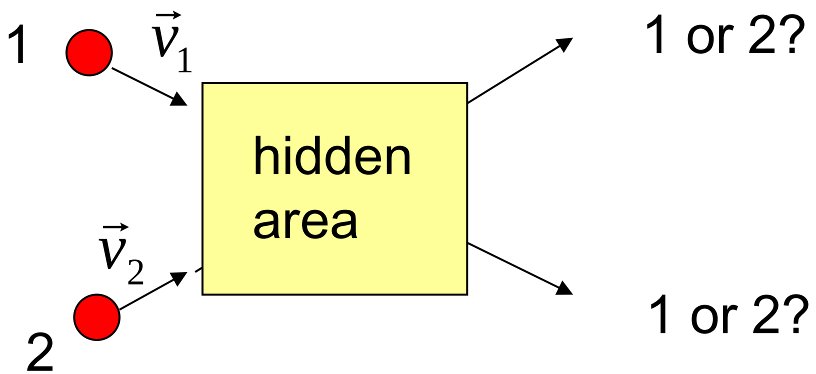
e.g. Two electrons in the Helium atom. All electrons are identical.

This introduces a complication in quantum mechanics that does not exist in classical physics.

In classical mechanics we can always, in principle, distinguish between two particles even if they are identical.

Let us take the example of two identical billiard balls.

We direct them so that there is a possibility that they will collide.



Two Particle Systems

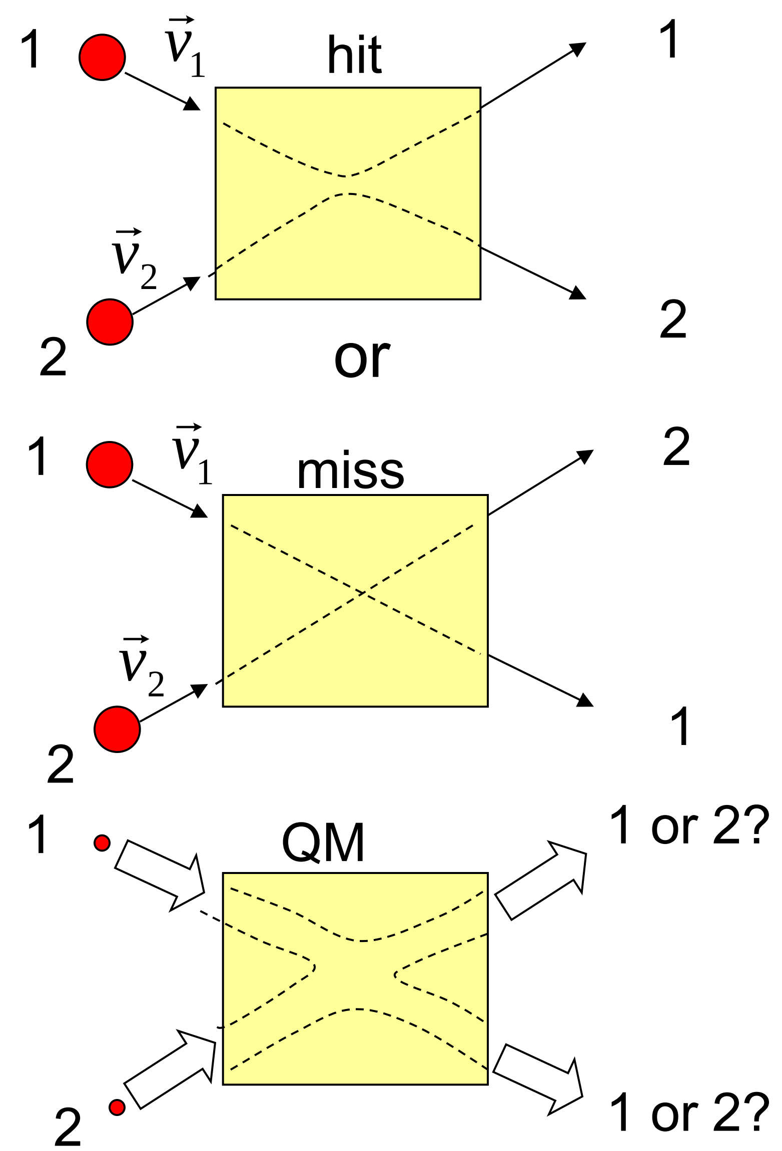
In classical physics, if we know the initial positions and velocities of the balls we can predict with certainty the path they will take.

So in classical physics the particles are distinguishable.

- We can keep track of what an individual particle does – even if we cannot see it.

But, in Quantum Mechanics, the Heisenberg Uncertainty principle prevents us from doing this.

- If we put two identical particles in a small space we cannot follow what an individual particle does.



Two Particle Systems

So, in Quantum Mechanics, identical particles are indistinguishable.

e.g. If an atom has two electrons in it, we cannot tell which electron is in which single particle state.

Returning to our 1-dimensional example:

In the two-particle wave function $\psi(x_1, x_2)$,

if the two particles are identical, there is no way to tell which particle is at position x_1 and which is at x_2.

Therefore the probability distribution $|\psi(x_1, x_2)|^2$ must be physically indistinguishable from $|\psi(x_2, x_1)|^2$.

i.e. the probability distribution for identical particles must be independent of interchanging the labels x_1 and x_2.

Two Particle Systems

So for identical particles we must have

$$|\psi(x_1, x_2)|^2 = |\psi(x_2, x_1)|^2$$

Therefore:

either $\psi(x_2, x_1) = +\psi(x_1, x_2)$

Symmetric with respect to exchange.

or $\psi(x_2, x_1) = -\psi(x_1, x_2)$

Anti-Symmetric with respect to exchange.

Two Particle Systems

Let us take a specific example to illustrate the consequences of this exchange symmetry requirement for identical particles.

Suppose we have two identical, non-interacting, particles moving in a 1-dimensional infinite square well.

Let $\psi_{n,m}(x_1, x_2)$ be the wave function where one of the particles is in the single particle state with quantum number n and the other is in the single particle sate with quantum number m.

Such a state could be $\psi_{n,m}(x_1, x_2) = \psi_n(x_1)\psi_m(x_2)$

Note that in this state we are explicitly saying that particle 1 is in state n and particle 2 is in state m.

(In QM this is a problem…we cannot know that!)

Two Particle Systems

$$\psi_1 = \sqrt{\frac{2}{a}}\sin\left(\frac{\pi}{a}x\right)$$
$$\psi_2 = \sqrt{\frac{2}{a}}\sin\left(\frac{2\pi}{a}x\right)$$

Let us be more specific and let $n = 1$ and $m = 2$.

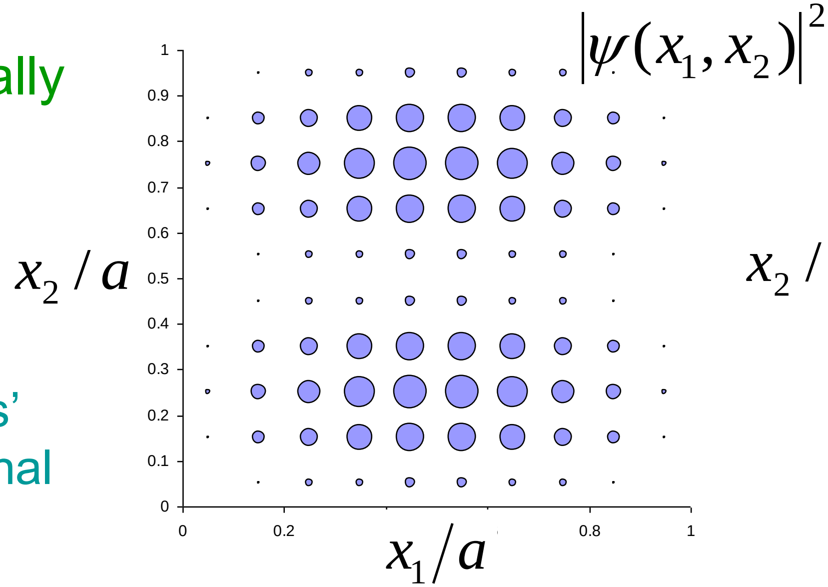
So $$\psi(x_1, x_2) = \frac{2}{a}\sin\left(\frac{\pi}{a}x_1\right)\sin\left(\frac{2\pi}{a}x_2\right)$$

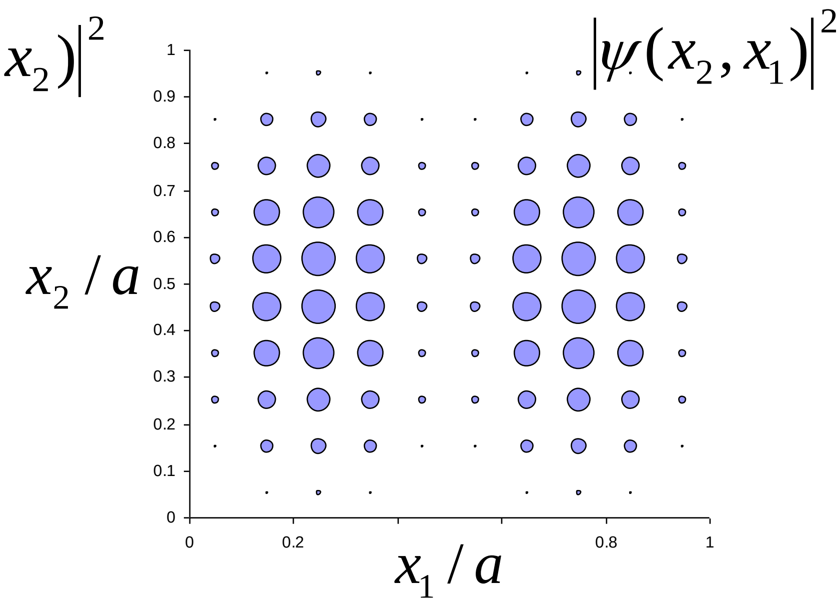
If we interchange x_1 and x_2 we get

$$\psi(x_2, x_1) = \frac{2}{a}\sin\left(\frac{\pi}{a}x_2\right)\sin\left(\frac{2\pi}{a}x_1\right)$$

We see that $|\psi(x_1, x_2)|^2 \neq |\psi(x_2, x_1)|^2$

Graphically





The size of the 'bubbles' is proportional to $|\psi|^2$.

Two Particle Systems

Therefore, since $|\psi(x_1, x_2)|^2 \neq |\psi(x_2, x_1)|^2$

the wave function $\psi_{n,m}(x_1, x_2) = \psi_n(x_1)\psi_m(x_2)$

– although it is a solution to the SE – cannot be the correct wave function for the two particle system.

We know that linear combinations of solutions to the SE are also solutions. Some of these will satisfy the exchange symmetry.

i.e. satisfy $|\psi(x_1, x_2)|^2 = |\psi(x_2, x_1)|^2$

The solutions also need to have the same total energy as

$$\psi_{n,m}(x_1, x_2) = \psi_n(x_1)\psi_m(x_2)$$

Because exchanging identical particles cannot change the energy.

So the correct solutions must be linear combinations of

$\psi_n(x_1)\psi_m(x_2)$ and $\psi_n(x_2)\psi_m(x_1)$

Two Particle Systems

The linear combinations that satisfy the criteria are:

Symmetric wave function:

$$\psi_S(x_1,x_2)=\frac{1}{\sqrt{2}}\left[\psi_n(x_1)\psi_m(x_2)+\psi_n(x_2)\psi_m(x_1)\right]$$

which has $\psi_S(x_1,x_2)=+\psi_S(x_2,x_1)$

Anti-Symmetric wave function:

$$\psi_A(x_1,x_2)=\frac{1}{\sqrt{2}}\left[\psi_n(x_1)\psi_m(x_2)-\psi_n(x_2)\psi_m(x_1)\right]$$

which has $\psi_A(x_1,x_2)=-\psi_A(x_2,x_1)$

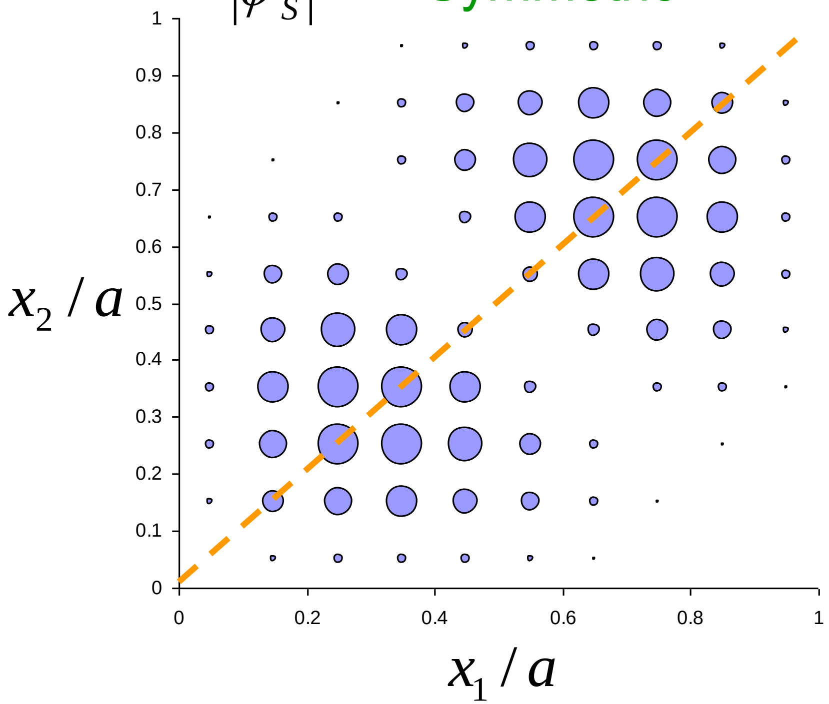
The factor of $\frac{1}{\sqrt{2}}$ comes from preserving the normalization.

i.e. $\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\left|\psi_{S,A}(x_1,x_2)\right|^2 dx_1 dx_2=1$ where the single particle wave functions are normalized. $\int_{-\infty}^{\infty}\left|\psi_n(x)\right|^2 dx=1$

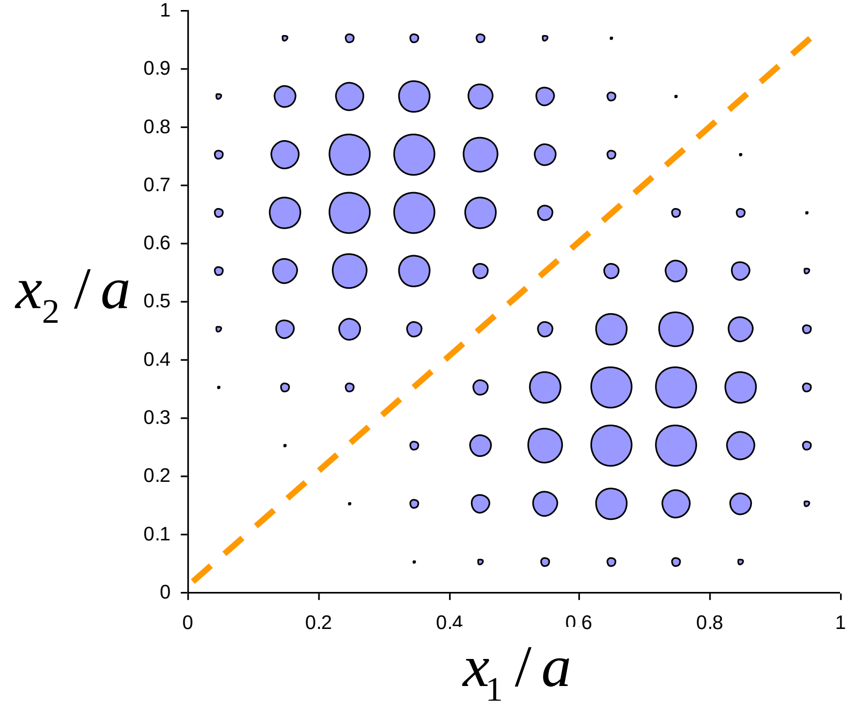
Two Particle Systems

Probability distributions for the example $n = 1$ and $m = 2$.

$|\psi_S|^2$ Symmetric



$|\psi_A|^2$ Anti-Symmetric



Particles cluster together along the line $x_1 = x_2$.

Particles are never near each other.

Indeed $|\psi_A|^2 = 0$ when $x_1 = x_2$

Two Particle Systems

Note: The clustering of the particles (in the symmetric case) or the anti-clustering (in the anti-symmetric case) has nothing to do with any forces between the particles.

Remember we are considering non-interacting particle in this example.

Furthermore:

If the particles are in the same single particle state,

For the symmetric state:

$$n = m \quad \Rightarrow \psi_S(x_1, x_2) \quad \text{is finite,}$$

But for the anti-symmetric state:

$$n = m \;\Rightarrow\; \psi_A(x_1, x_2) = \frac{1}{\sqrt{2}}\left[\psi_n(x_1)\psi_n(x_2) - \psi_n(x_2)\psi_n(x_1)\right]$$

$$\Rightarrow \psi_A(x_1, x_2) = 0 \;\; \text{always.}$$

No particles at all!

Two Particle Systems

To summarize, for identical particles:

If the system is in a Symmetric state:
- the particles tend to be near each other.
- the particles can be in the same quantum state.

If the system is in an Anti-Symmetric state:
- the particles do not like to be near each other.
- the particles cannot be in the same quantum state.

What determines what kind of state the system can be in?

It depends on the type of particles in the system.

In fact it depends on the intrinsic spin of the particles.

Two Particle Systems

We now know that a complete description of the state of a particle must include the spin state of the particle.

The total wave function for particle 1 can be written

$$\psi_{Tot}(1) = \psi(\vec{r}_1)\chi(1)$$

Space part

Spin part

Depends on the quantum numbers n, l & m_l in an atom for example.

We do not know what coordinate this depends on. But we do know that the spin state of the particle is specified by the quantum number m_s.

For an electron $m_s = +\frac{1}{2}$ or $-\frac{1}{2}$

For clarity I will write: $\chi_{m_s=\frac{1}{2}}(1) = \alpha(1)$ "Spin up" state

$\chi_{m_s=-\frac{1}{2}}(1) = \beta(1)$ "Spin down" state

Two Particle Systems

For two electrons the total wave function will be

$$\psi_{Tot}(1,2) = \psi(\vec{r}_1, \vec{r}_2)\chi(1,2)$$

Total space wave function will be symmetric or anti-symmetric.

Two electron spin state

The total wave function must have a probability distribution that is indistinguishable when we exchange the particle coordinates,

i.e. $$|\psi_{Tot}(1,2)|^2 = |\psi_{Tot}(2,1)|^2$$

$$\Rightarrow |\psi(\vec{r}_1, \vec{r}_2)\chi(1,2)|^2 = |\psi(\vec{r}_2, \vec{r}_1)\chi(2,1)|^2$$

So the product $\psi(\vec{r}_1, \vec{r}_2)\chi(1,2) = \pm\psi(\vec{r}_2, \vec{r}_1)\chi(2,1)$

Now since $\psi(\vec{r}_1, \vec{r}_2) = \pm\psi(\vec{r}_2, \vec{r}_1)$ $\quad \Rightarrow \chi(1,2) = \pm\chi(2,1)$

What restrictions does this place on $\chi(1,2)$?

Two Particle Systems

Since there are only two spin states of an electron, we can write down all the possible forms for $\chi(1,2)$.

$$\chi(1,2) = \alpha(1)\beta(2)$$

$$\chi(1,2) = \beta(1)\alpha(2)$$

Neither symmetric nor anti-symmetric

So these cannot be correct solutions to the system.

$$\chi(1,2) = \alpha(1)\alpha(2)$$ Symmetric

$$\chi(1,2) = \beta(1)\beta(2)$$ Symmetric

We can construct symmetric and anti-symmetric states from the first two (we know that linear combinations of solutions to a quantum system are also solutions).

$$\chi_S(1,2) = \frac{1}{\sqrt{2}}\left[\alpha(1)\beta(2) + \alpha(2)\beta(1)\right]$$ Symmetric

$$\chi_A(1,2) = \frac{1}{\sqrt{2}}\left[\alpha(1)\beta(2) - \alpha(2)\beta(1)\right]$$ Anti-Symmetric

Two Particle Systems

Therefore there are 4 possible total spin states for the two electrons.

These correspond to the 4 possible total spin quantum numbers.

Symmetric States $S=1$ Triplet Spins “Aligned”

$$\chi_S(1,2)=\alpha(1)\alpha(2) \qquad m_S=+1$$

$$\chi_S(1,2)=\frac{1}{\sqrt{2}}\left[\alpha(1)\beta(2)+\alpha(2)\beta(1)\right] \qquad m_S=0$$

$$\chi_S(1,2)=\beta(1)\beta(2) \qquad m_S=-1$$

Anti-Symmetric State $S=0$ Singlet Spins “Anti-Aligned”

$$\chi_A(1,2)=\frac{1}{\sqrt{2}}\left[\alpha(1)\beta(2)-\alpha(2)\beta(1)\right] \qquad m_S=0$$

Two Particle Systems

Now since $\psi_{Tot}(1,2) = \psi(\vec{r}_1, \vec{r}_2)\chi(1,2)$

must be either symmetric or anti-symmetric.

The symmetric states are $\psi_{Tot,S} = \psi_S \chi_S$

or $\psi_{Tot,S} = \psi_A \chi_A$

The anti-symmetric states are $\psi_{Tot,A} = \psi_S \chi_A$

or $\psi_{Tot,A} = \psi_A \chi_S$

Now, in Nature we find that, if the two particles are:

Fermions $\Rightarrow$ The total wave function is always anti-symmetric

Bosons $\Rightarrow$ The total wave function is always symmetric

Why? – Relativity provides the connection between spin and the Fermions and Bosons of Statistical Mechanics.

Two Particle Systems

Electrons are Fermions.

Therefore atoms must have total wave functions that are anti-symmetric.

If the two electrons have their spins aligned,

i.e. They are in one of the symmetric triplet, $S = 1$ states,

They have the same individual m_s quantum number.

then since $\psi_{Tot,A} = \psi_A \chi_S$

$\Rightarrow \psi(\vec{r}_1, \vec{r}_2)$ must be anti-symmetric

Therefore, the two electrons cannot have the same set of space quantum numbers, n, l & m_l.

Two Particle Systems

Electrons are Fermions.

Therefore atoms must have total wave functions that are anti-symmetric.

If the two electrons have their spins anti-aligned,

i.e. They are in the anti-symmetric singlet, $S = 0$ state,

They have the different individual m_s quantum numbers.

then since $\psi_{Tot,A} = \psi_S \chi_A$

$\Rightarrow \psi(\vec{r}_1, \vec{r}_2)$ must be symmetric

Therefore, the two electrons can have the same set of space quantum numbers, n, l & m_l.

Two Particle Systems

These observations lead to the

Pauli Exclusion Principle for atoms

No two electrons in the same atom can have all four quantum numbers the same.

This implies that:

In each "space" state, specified by n, l & m_l, there can be only two electrons ($m_s = \pm\frac{1}{2}$).

Similar statements apply to nucleons in a nucleus.

We will find many more applications…

e.g. in the quark model of particles.

Exchange Symmetry

The generalization that will be important for us is:

In a multi-particle system, the exchange of any two identical fermions must be anti-symmetric.

i.e. the sign of the <u>total</u> wave function of the system must change.

In a multi-particle system, the exchange of any two identical bosons must be symmetric.

i.e. the sign of the <u>total</u> wave function of the system must not change.