

EXCHANGE FORCES

Let us imagine to have a system of two particles in states (a) and (b), respectively. The 2-particle wavefunction will be:

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

If the two particles are indistinguishable, relativity and spin-statistic theorem tell us that we have two possibilities:

1 and 2 are identical fermions (semi-integer spin): $\psi(\vec{r}_1, \vec{r}_2) = \frac{1}{\sqrt{2}} (\psi_a(\vec{r}_1) \psi_b(\vec{r}_2) - \psi_b(\vec{r}_1) \psi_a(\vec{r}_2))$

1 and 2 are identical bosons (integer spin): $\psi(\vec{r}_1, \vec{r}_2) = \frac{1}{\sqrt{2}} (\psi_a(\vec{r}_1) \psi_b(\vec{r}_2) + \psi_b(\vec{r}_1) \psi_a(\vec{r}_2))$

Let us look at the average distance between the two particles:

$$\langle |\vec{r}_1 - \vec{r}_2|^2 \rangle = \iint d^3\vec{r}_1 d^3\vec{r}_2 \psi^*(\vec{r}_1, \vec{r}_2) |\vec{r}_1 - \vec{r}_2|^2 \psi(\vec{r}_1, \vec{r}_2)$$

Let us also move to a 1-D world to simplify the notation: $\vec{r} \rightarrow x$

$$\langle (x_1 - x_2)^2 \rangle = \langle x_1^2 \rangle + \langle x_2^2 \rangle - 2 \langle x_1 x_2 \rangle$$

$$\langle x_1^2 \rangle = \iint dx_1 dx_2 \frac{1}{\sqrt{2}} (\psi_a^*(x_1) \psi_b^*(x_2) \pm \psi_a^*(x_2) \psi_b^*(x_1)) x_1^2 \frac{1}{\sqrt{2}} (\psi_a(x_1) \psi_b(x_2) \pm \psi_a(x_2) \psi_b(x_1))$$

$$= \iint dx_1 dx_2 \frac{1}{2} |\psi_a(x_1)|^2 |\psi_b(x_2)|^2 x_1^2 +$$

$$+ \iint dx_1 dx_2 \frac{1}{2} |\psi_a(x_2)|^2 |\psi_b(x_1)|^2 x_1^2 +$$

$$\pm \iint dx_1 dx_2 \frac{1}{2} \psi_a^*(x_1) \psi_a(x_2) x_1^2 \psi_b^*(x_2) \psi_b(x_1) +$$

$$\pm \iint dx_1 dx_2 \frac{1}{2} \psi_a^*(x_2) \psi_a(x_1) x_1^2 \psi_b^*(x_1) \psi_b(x_2)$$

All good so far, but we saw that, at least in the case of fermions, $\psi_a(\vec{r}) \neq \psi_b(\vec{r})$, otherwise $\psi(\vec{r}_1, \vec{r}_2) = 0$ (Pauli's exclusion principle). Let us then take our two identical particles to be in two different and orthogonal states. Typical situation: two electrons in different orbital states. Then:

$$\langle X_1^2 \rangle = \frac{1}{2} (\langle X_1^2 \rangle_a + \langle X_1^2 \rangle_b)$$

Here's how (back to page before):

$$\langle X_1^2 \rangle_a = \int dx_1 |\psi_a|^2 X_1^2 \underbrace{\int dx_2 |\psi_b(x_2)|^2}_1$$

$$\langle X_1^2 \rangle_b = \underbrace{\int dx_2 |\psi_a(x_2)|^2}_1 \int dx_1 |\psi_b(x_1)|^2 X_1^2$$

$$\int dx_2 \psi_b^*(x_2) \psi_a(x_2) = 0 \Rightarrow \text{third term in sum} = 0$$

$$\int dx_2 \psi_a^*(x_2) \psi_b(x_2) = 0 \Rightarrow \text{fourth term in sum} = 0$$

The same calculations must apply for $\langle X_2^2 \rangle$, after all the two particles are indistinguishable. What about $\langle X_1 X_2 \rangle$?

$$\begin{aligned} \langle X_1 X_2 \rangle &= \frac{1}{2} \int dx_1 \int dx_2 (\psi_a^*(x_1) \psi_b^*(x_2) \pm \psi_a^*(x_2) \psi_b^*(x_1)) X_1 X_2 (\psi_a(x_1) \psi_b(x_2) \pm \psi_a(x_2) \psi_b(x_1)) \\ &= \frac{1}{2} \int dx_1 \psi_a^*(x_1) X_1 \psi_a(x_1) \int dx_2 \psi_b^*(x_2) X_2 \psi_b(x_2) + \\ &\quad + \frac{1}{2} \int dx_1 \psi_b^*(x_1) X_1 \psi_b(x_1) \int dx_2 \psi_a^*(x_2) X_2 \psi_a(x_2) + \\ &\quad \pm \frac{1}{2} \int dx_1 \psi_a^*(x_1) X_1 \psi_b(x_1) \int dx_2 \psi_b^*(x_2) X_2 \psi_a(x_2) + \\ &\quad \pm \frac{1}{2} \int dx_1 \psi_b^*(x_1) X_1 \psi_a(x_1) \int dx_2 \psi_a^*(x_2) X_2 \psi_b(x_2) \end{aligned}$$

$$2\langle X_1, X_2 \rangle = \langle X_1 \rangle_a \langle X_2 \rangle_b + \langle X_2 \rangle_a \langle X_1 \rangle_b + \\ \pm \langle X_1 \rangle_{ab} \langle X_2 \rangle_{ba} \pm \langle X_2 \rangle_{ab} \langle X_1 \rangle_{ba}$$

Two notes: 1) $\langle X_1 \rangle_a = \langle X_2 \rangle_a$: indistinguishable particles
 $\langle X_1 \rangle_b = \langle X_2 \rangle_b$

2) $\langle X \rangle_{ab} = \langle X \rangle_{ba}^*$: check integral definitions

Therefore, putting everything together:

$$\langle X_1, X_2 \rangle = \langle X \rangle_a \langle X \rangle_b \pm |\langle X \rangle_{ab}|^2$$

Finally:

$$\langle |X_1 - X_2|^2 \rangle = \langle X^2 \rangle_a + \langle X^2 \rangle_b - 2\langle X \rangle_a \langle X \rangle_b \mp 2|\langle X \rangle_{ab}|^2$$

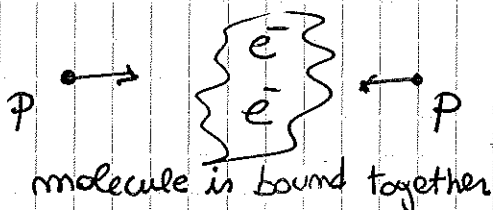
Bosons feel an effective "exchange force" pushing them together, while fermions feel an effective "exchange force" pushing them apart:

$$\langle |X_1 - X_2|^2 \rangle_{\text{bosons}} < \langle |X_1 - X_2|^2 \rangle_{\text{fermions}}$$

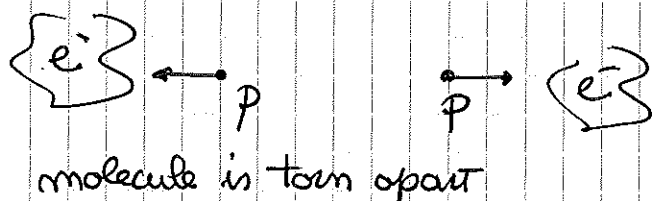
Exchange force is purely geometrical consequence of symmetry requirement.

Let us consider a H_2 molecule. Let us consider what happens if our electrons (a pair of identical fermions) are in a symmetric spatial configuration, or in an anti-symmetric spatial configuration:

symmetric: they tend to stay close to each other



anti-symmetric: exchange force tends to push them apart



Did we just prove that the H_2 molecule cannot exist?

Hard to believe. The fact is that we need to consider the complete state of the system, which includes spin: the state of an electron is $\psi(\vec{r}) \cdot \chi(\vec{S})$ [technically, S_z only: I know $S^2 = 3\hbar^2/4$].

Then, my 2-electron state can be written in such a way that it is spatially symmetric and spin anti-symmetric. The total state becomes anti-symmetric, and it is acceptable for a pair of identical fermions.

How do I write an anti-symmetric spin state?

$$\begin{aligned} \frac{\chi_1(+\hbar/2)\chi_2(-\hbar/2) - \chi_1(-\hbar/2)\chi_2(+\hbar/2)}{\sqrt{2}} &= \frac{|\frac{1}{2} \frac{1}{2}\rangle |\frac{1}{2} -\frac{1}{2}\rangle - |\frac{1}{2} -\frac{1}{2}\rangle |\frac{1}{2} \frac{1}{2}\rangle}{\sqrt{2}} \\ &= |0 \ 0\rangle \quad S_z = S_{z1} + S_{z2} \\ &\quad \uparrow \vec{S} = \vec{S}_1 + \vec{S}_2 \end{aligned}$$

Indeed, chemists measure that the two electrons in a H_2 molecule are in a state with total spin = 0.

Example of exchange force: neutron stars. Very heavy (estimate density of neutrons tightly together to density of matter, in which $r_{\text{proton}} \sim 1 \text{ fm} = 10^{-15} \text{ m}$ and $r_{\text{atom}} \sim 1 \text{ \AA} = 10^{-10} \text{ m}$), the gravitational pull towards collapse is balanced by the exchange force: neutrons are fermions and don't like being pulled too close together.