But $\hat{P}|a_1\rangle|b_2\rangle = |a_2\rangle|b_1\rangle \neq -|a_1\rangle|b_2\rangle$

in 1930 Fock discovered a simple solution

If $|a_1\rangle|b_2\rangle$ is an eigenfunction of $\hat{H}$, so is $|a_2\rangle|b_1\rangle$ since e^- are identical particles. $\Rightarrow$ let

normalization

$$\psi(1,2) \hat{=} \frac{1}{\sqrt{2}}|a_1\rangle|b_2\rangle - \frac{1}{\sqrt{2}}|a_2\rangle|b_1\rangle$$

$$\hat{=} \frac{1}{\sqrt{2}}\begin{vmatrix} |a_1\rangle & |b_1\rangle \\ |a_2\rangle & |b_2\rangle \end{vmatrix}$$ <u>Slater determinant</u>

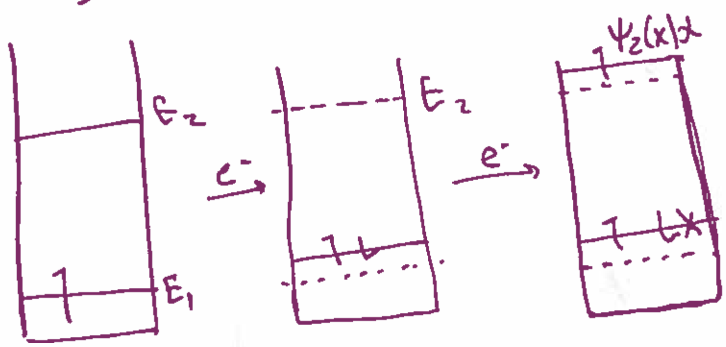
$$\hat{=} \hat{A}_2 |a_1\rangle|b_2\rangle$$

Now $\hat{P}\psi(1,2) = \frac{1}{\sqrt{2}}(|a_2\rangle|b_1\rangle) - \frac{1}{\sqrt{2}}|a_1\rangle|b_2\rangle = -\psi(1,2)$

We can now prove one of the most important principles of QM in chemistry:

"Two e^- cannot occupy the same state" $\boxed{\text{Pauli Exclusion}}$

Filling PIB w/ e^-



Postulate 6: quantum particles have an intrinsic angular momentum, called <u>spin</u>

$$\Rightarrow \psi_{e^-}(r, \theta, \varphi, \varphi_s) \sim R_{n\ell}(r) \cdot P_{\ell m}(\theta) \cdot e^{im_\ell \varphi} \cdot e^{\pm 1/2\, \varphi_s}$$

rotation of electron around itself- kinda

$s = \frac{1}{2}$ $m_s = \pm\frac{1}{2}$

can have different values, but that wouldn't be an electron (for example photon=1)

by Analogy

$Fe_{q=2}O_{s=3}$ is rust

if $s=0$; Fe metal

same way w/ physics elementary particle

[Dirac eq.] (relatively few relativistic effects, not too important for this class) (can't derive (in this class))

proper derivation

Classical analogy:

$s = 1/2$ $m_s = 1/2$ "α" $\vec{s}$ $s = 1/2$ $m_s = -1/2$ "β" $\vec{s}$

Rotating (-) charge produces a mag field

e^- has a weak magnetic field

In short, we can write the wave function of a single e^- (#1) in state "a" as

$$\left.\begin{matrix}\psi_a(x_1, y_1, z_1) \\ \psi_a(r_1, \theta_1, \varphi_1)\end{matrix}\right\} \cdot \left\{\begin{matrix}\alpha(\text{up}) \\ \beta(\text{down})\end{matrix}\right. \xrightarrow{\text{abbreviate}} |a_1\rangle$$

$|s\alpha$

e^- #1

- 'ket' notation
- we'll use it more
- QM & Linear algebra
  - derivation in a much shorter notation

<u>What about ψ for $2e^-$</u>

Consider the simplest case: e^- are far apart

$$\psi_{(1,2)} = |a_1\rangle |b_2\rangle$$

Postulate 6: $s = 1/2 = e^-$ is a Fermion

$$\hat{P}\psi(1,2) = \psi(2,1) = -\psi(1,2)$$

$\hat{P}$ switches e^- #1 & e^- #2

if + you would not be able to form chemical bonds