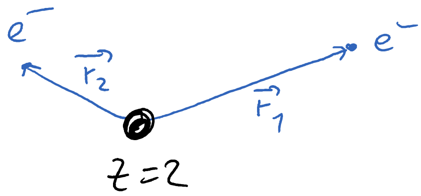
Donnerstag, 25. November 2021 13:15

The Helium Atom



$$H = \overbrace{\frac{p_1^2}{2m} - \frac{Ze^2}{4\pi\varepsilon_0}\cdot\frac{1}{r_1}}^{H} + \underbrace{\frac{p_2^2}{2m} - \frac{Ze^2}{4\pi\varepsilon_0}\cdot\frac{1}{r_2}}_{H} + \underbrace{\frac{e^2}{4\pi\varepsilon_0}\,\frac{1}{|\vec{r}_1-\vec{r}_2|}}_{\text{e-e interaction}}$$

What we will <u>neglect</u> for now

+ relativistic effects
+ spin - angular momentum coupling $l_1 s_1$, $l_2 s_2$
+ „crossed" — " — $l_1 s_2$, $l_2 s_1$
+ spin-spin coupling
+ momentum - momentum coupling $l_1 l_2$

Calculate spectrum, state by state

we treat e-e Coulomb interaction as weak perturbation

↳ perturbation theory

Total wave function for He

Spin statistics theorem

- Fermions have antisymmetric total w.f. w.r.t. the exchange of 2 particles

  $\Rightarrow$ w.f. changes sign when 2 particles are exchanged

- Bosons have symmetric total w.f.

$$\Psi_{ges} = u_{a,s}(\vec{r}_1, \vec{r}_2) \cdot \chi_{s,a}$$

Either spatial w.f. is antisymmetric

$\rightarrow$ then spin w.f. is symmetric

or vice versa

<u>Spin w.f.</u> $\chi_{s,a}$

Couple 2 spin $1/2$ particles

Triplett states $S=1$

$$|S=1, M_s=+1\rangle = \uparrow_1 \uparrow_2$$

$$|S=1, M_s=0\rangle = \frac{1}{\sqrt{2}}\left(\uparrow_1\downarrow_2 + \downarrow_1\uparrow_2\right)$$

$$|S=1, M_s=-1\rangle = \downarrow_1\downarrow_2$$

Symmetric spin wave functions

no sign change w.r.t. particle exchange

Singlet state $S=0$

$$|S=0, M_s=0\rangle = \frac{1}{\sqrt{2}}\left(\uparrow_1\downarrow_2 - \downarrow_1\uparrow_2\right)$$

anti-symmetric

changes sign when you exchange

particles

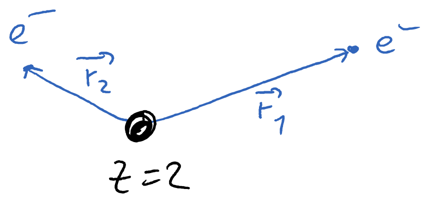
Anti-symmetric total w.f.

Spatial w.f. $\quad u_{n_1,l_1,m_1}(\vec r_1) \equiv u_{q_1}(\vec r_1)$

$$u_{n_2 l_2 m_2}(\vec r_2) \equiv u_{q_2}(\vec r_2)$$

exchange of the 2 electrons

$\hat{=} \quad \vec r_1 \leftrightarrow \vec r_2 \qquad$ (obvious)



symmetric spatial w.f.:

$$u_s(\vec r_1, \vec r_2) = \frac{1}{\sqrt{2}}\left(u_{q_1}(1)\, u_{q_2}(2) + u_{q_1}(2)\, u_{q_2}(1)\right)$$

$$\downarrow$$

$$-$$

anti-symmetric

$$u_a(\vec r_1, \vec r_2) =$$

side remark Impact of antisymmetric w.f. : Pauli principle

associated spatial probability distribution

$$|u_a(\vec r_1, \vec r_2)|^2 = \left|\frac{1}{\sqrt{2}}\left(u_{q_1}(1)\, u_{q_2}(2) - u_{q_1}(2)\, u_{q_2}(1)\right)\right|^2$$

$$= 0 \quad \text{if} \quad \vec r_1 = \vec r_2$$

u_a antisymmetric spatial w.f.

is associated with

χ_s symmetric spin w.f.

$$\text{e.g. } |S=1, M_S=1\rangle = \uparrow_1 \uparrow_2$$

$\Rightarrow$ total w.f. = zero for 2 spins $\uparrow\uparrow$ and same $\vec{r}$

2 parallel spins can not be in the same place

Pauli blockade