Identical particles (Ch. 12)

- 2 particles are identical if there is no intrinsic way of telling them apart.

- They can have different dynamical properties, such as positions, momenta, and components of spin, but their invariant properties, such as their $\hat{S}^2$ spin quantum number "s", as well as mass and charge, are the same.

- There are therefore no additional invariant properties that can be used to distinguish identical particles from each other as they move and interact.
  In other words, there is no way *in principle* to "mark" one as "particle number 1" and another as "particle number 2".

- We have discovered that at the atomic and sub-atomic level, nature is made up of identical particles in this sense.

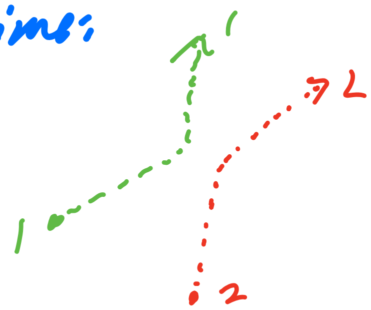
Their existence is some sort of indication that we are approaching a more "fundamental" description of nature.

- Examples:

  e^- : all electrons have $s = 1/2$, $q = -e$, $m = 0.511\ldots$ MeV

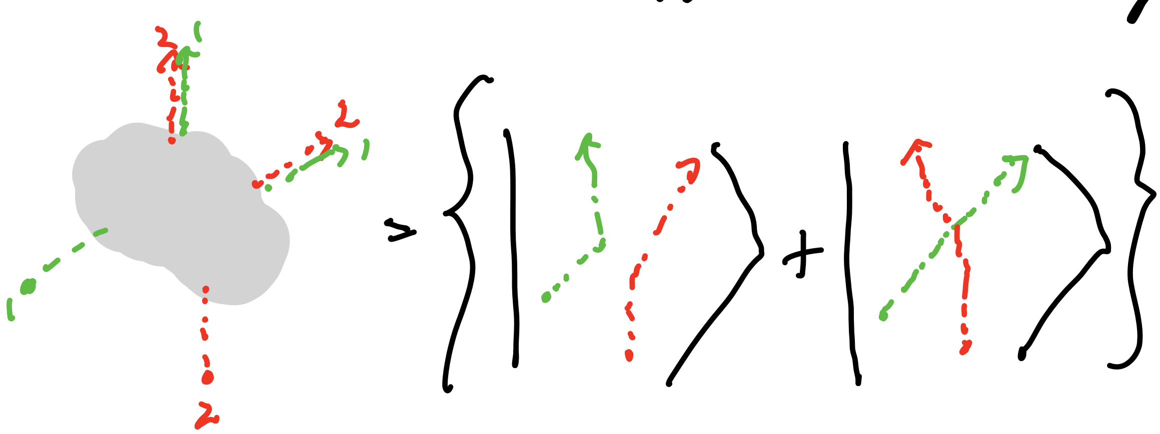
  H : all hydrogen atoms in their ground state are all identical. But 2 H-atoms in different internal energy eigenstates are distinguishable.

- In classical mechanics can tell apart by following position in time:



Thus, even if we accept that the two particles are identical in the above sense, we could still label them by their initial positions.

- In QM, there are no definite paths, so can't use this strategy to tell them apart:



So the existence of identical particles is an inherently quantum phenomenon.

- If 2 particles are distinguishable then

$$\begin{cases} \text{particle } 1 \leftrightarrow \text{Hilbert space } \#1 \equiv V_1 \\ \quad " \quad\;\; 2 \leftrightarrow \quad " \qquad " \quad\; \#2 \equiv V_2 \end{cases}$$

and total 2-particle state is

$$|\psi\rangle \in V_1 \otimes V_2 .$$

E.g., if $|\psi_1\rangle = |x_1 = a\rangle$, $\hat{x}$ eigenstate in V_1
& $|\psi_2\rangle = |x_2 = b\rangle$, $\hat{x}$ " " V_2

$$\Rightarrow \quad |\psi\rangle = |a\rangle \otimes |b\rangle \doteq |a, b\rangle$$

& $|\psi\rangle = |b, a\rangle$ is a different state.

- But if particles are identical, then

$$V_1 \simeq V_2$$

"isomorphic" = "same shape"

and can't tell $|a, b\rangle$ & $|b, a\rangle$ apart.

$\Rightarrow$ Rule: For identical particles, state remains the same under interchange of their "labels" $1 \leftrightarrow 2$.

- How do we implement this mathematically? Although $V_1 \otimes V_2 \simeq V_1 \otimes V_1 \simeq V_2 \otimes V_1$, we still have that $|a, b\rangle \neq |b, a\rangle$.

Say $|\psi\rangle = \alpha\, |a, b\rangle + \beta\, |b, a\rangle$.
Interchange $1 \leftrightarrow 2$ labels, get new state

$$\alpha |b, a\rangle + \beta |a, b\rangle \overset{?}{=} |\psi\rangle$$

Only invariant if $\alpha = \beta$, i.e., if

$$|\psi\rangle = \alpha \underbrace{\left(|ab\rangle + |ba\rangle\right)}_{\text{"symmetrized state"}}$$

- But $|\psi\rangle$ and $e^{i\theta}|\psi\rangle$ are physically equivalent for any θ, so there are more possibilities:

$$e^{i\theta}|\psi\rangle = \alpha\, |b, a\rangle + \beta |a, b\rangle$$

$$\Rightarrow \quad \alpha = \beta e^{i\theta} \quad \& \quad \beta = \alpha e^{i\theta}$$

$$\Rightarrow \quad e^{2i\theta} = 1 \quad \Rightarrow \quad e^{i\theta} = \pm 1.$$

$e^{i\theta} = +1$: $\alpha = \beta \Rightarrow |\psi\rangle \propto |ab\rangle + |ba\rangle$ symmetrized

$e^{i\theta} = -1$: $\alpha = -\beta \Rightarrow |\psi\rangle \propto |ab\rangle - |ba\rangle$ antisymmetrized

- $\boxed{\begin{array}{l}\text{"Bosons"} \doteq \text{identical particles which have symmetrized states.} \\ \text{"Fermions"} \doteq \text{identical particles which have antisymmetrized states.}\end{array}}$

The "statistics" of a particle refers to whether it is a boson or a fermion. Hence "Bose-Einstein statistics" or "Fermi-Dirac statistics".

- 2 distinguishable particles with same spin have same Hilbert space, V. So

$V \otimes V$ = 2-particle Hilb. space if distinguishable

$$V \otimes V = \underset{\substack{\uparrow \\ \text{bosons}}}{V_S} \oplus \underset{\substack{\uparrow \\ \text{fermions}}}{V_A}$$

V_S = 2-particle Hilb. sp. of identical bosons

V_A = 2-particle Hilb. sp. of identical fermions

V_S & V_A are orthogonal subspaces of $V \otimes V$

$$\begin{array}{ccc} V_S & & V_A \\ \rotatebox{90}{$\in$} & & \rotatebox{90}{$\ni$} \\ |S\rangle \doteq |ab\rangle + |ba\rangle & & |cd\rangle - |dc\rangle \doteq |A\rangle \end{array}$$

$$\begin{aligned}
\Rightarrow \langle S|A\rangle &= \left(\langle ab| + \langle ba|\right)\left(|cd\rangle - |dc\rangle\right) \\
&= \langle ab|cd\rangle + \langle ba|cd\rangle - \langle ab|dc\rangle - \langle ba|dc\rangle \\
&= \cancel{\langle a|c\rangle\langle b|d\rangle} + \cancel{\langle b|c\rangle\langle a|d\rangle} \\
&\quad - \cancel{\langle a|d\rangle\langle b|c\rangle} - \cancel{\langle b|d\rangle\langle a|c\rangle} \\
&= 0
\end{aligned}$$

no matter what $|a\rangle, |b\rangle, |c\rangle, |d\rangle \in V$.

- Note: not every state in V_S or V_A can be written as

$$|\psi\rangle = |a, b\rangle \pm |b, a\rangle$$

For example

$$|\psi\rangle = \left(|ab\rangle + |cd\rangle\right) \pm \left(|ba\rangle + |dc\rangle\right)$$

$$\neq \left(|a\rangle + |c\rangle\right)\left(|b\rangle + |d\rangle\right) \pm \left(|b\rangle + |d\rangle\right)\left(|a\rangle + |c\rangle\right)$$

This is the boson/fermion version of unentangled versus entangled states.

Orthonormal bases of V_A & V_S

- Say $\{|i\rangle,\ i=1\cdots n\}$ is o-n basis of V.
  Then $\{|i,j\rangle,\ i,j=1\cdots n\}$ " " " " $V\otimes V$.

- O-n basis V_S:

$$\left\{\begin{array}{ll} \frac{1}{\sqrt{2}}\left(|i,j\rangle + |j,i\rangle\right) & 1\le i<j\le n \\ |i,i\rangle & 1\le i\le n \end{array}\right\} \equiv \{|ij,S\rangle\}_{i\le j}$$

$$\Rightarrow \dim V_S = \tfrac{1}{2}n(n+1).$$

- O-n basis V_A:

$$\left\{ \frac{1}{\sqrt{2}}\left(|i,j\rangle - |j,i\rangle\right) \quad 1\le i<j\le n\right\} \equiv \{|ij,A\rangle\}_{i<j}$$

$$\Rightarrow \dim V_A = \tfrac{1}{2}n(n-1)$$

(Note: $\dim V_S + \dim V_A = n^2 = \dim(V\otimes V)$ ✓)

No "$|ii\rangle$" allowed ≡ "Pauli exclusion principle."

- Orthonormality & completeness:

V_S: $\langle ij, S | kl, S \rangle = \delta_{ik}\delta_{jl}$

$$\sum_{1 \le i \le j \le n} |ij, S\rangle\langle ij, S| = 1_S$$ identity on V_S not on $V \otimes V$!

V_A: $\langle ij, A | kl, A \rangle = \delta_{ik}\delta_{jl}$

$$\sum_{1 \le i < j \le n} |ij, A\rangle\langle ij, A| = 1_A$$ identity on V_A.

- Continuous basis: (eg 3-d position eigenbasis $|\vec{x}\rangle$)

Bosons:

$$|\vec{x}_1 \vec{x}_2, S\rangle \equiv \frac{1}{\sqrt{2}}\left(|\vec{x}_1 \vec{x}_2\rangle + |\vec{x}_2, \vec{x}_1\rangle\right) \qquad (*)$$

– No natural way to order "$\vec{x}_1 < \vec{x}_2$", so just accept that

$$|\vec{x}_1 \vec{x}_2, S\rangle = |\vec{x}_2 \vec{x}_1, S\rangle$$

are the same state, and be careful not to overcount!

- With ⊛ definition, get $|\vec{x}_1\vec{x}_1, S\rangle = \sqrt{2}\,|\vec{x}_1\vec{x}_1\rangle$ which has wrong normalization. We generally can just ignore this mistake bc it is wrong "in measure zero".

- Note that $\psi_S(\vec{x}_1,\vec{x}_2) = \psi_S(\vec{x}_2,\vec{x}_1)$.

$\Rightarrow$ orthonormality looks a bit different:

$$\langle \vec{x}_1\vec{x}_2, S | \vec{y}_1\vec{y}_2, S\rangle = \frac{1}{2}\left(\langle \vec{x}_1\vec{x}_2| + \langle \vec{x}_2\vec{x}_1|\right)\left(|\vec{y}_1\vec{y}_2\rangle + |\vec{y}_2\vec{y}_1\rangle\right)$$

$$= \delta^3(\vec{x}_1-\vec{y}_1)\,\delta^3(\vec{x}_2-\vec{y}_2) + \delta^3(\vec{x}_2-\vec{y}_1)\,\delta^3(\vec{x}_1-\vec{y}_2)$$

$\Rightarrow$ completeness needs factor of ½ to avoid over-counting:

$$\boxed{1_S = \frac{1}{2}\int d^3x_1\, d^3x_2\, |\vec{x}_1\vec{x}_2, S\rangle\langle \vec{x}_1\vec{x}_2, S|}$$

- Because of this factor of ½, we change the definition of wavefunction

$$\boxed{\psi_S(\vec{x}_1,\vec{x}_2) \doteq \frac{1}{\sqrt{2}}\langle \vec{x}_1\vec{x}_2, S|\psi_S\rangle} \quad *$$

$$= \frac{1}{\sqrt{2}}\cdot\frac{1}{\sqrt{2}}\left(\langle x_1 x_2| + \langle x_2 x_1|\right)|\psi_S\rangle$$

$$= \frac{1}{2}\left(\langle x_1 x_2 | \psi_S \rangle + \langle x_2 x_1 | \psi_S \rangle \right)$$

$$= \langle x_1 x_2 | \psi_S \rangle$$

using that $\langle x_1 x_2 | \psi_S \rangle = \langle x_2 x_1 | \psi_S \rangle$ since $|\psi_S\rangle$ is symmetrized.

- The normalization condition for ψ_S is

$$1 = \langle \psi_S | \psi_S \rangle = \langle \psi_S | 1_S | \psi_S \rangle$$

$$= \frac{1}{2} \int d^3x_1 d^3x_2 \, \langle \psi_S | x_1 x_2, S \rangle \langle x_1 x_2, S | \psi_S \rangle$$

$$= \int d^3x_1 d^3x_2 \, | \psi_S(\vec{x}_1, \vec{x}_2) |^2 .$$

- But note that since the 2 particles are identical, there is no way of telling which is at position x_1 and which at x_2, so the probability density

$$P(x_1, x_2) \doteq \begin{cases} \text{Probability}/(\text{vol})^2 \text{ to find} \\ \text{two particles at } x_1 \text{ \& } x_2 \end{cases}$$

is normalized by

$$1 = \int \frac{dx_1^3 \, dx_2^3}{2} P(x_1, x_2),$$

where the 2 factor corrects for integrating over both the (x_1, x_2) & the (x_2, x_1) configurations.

So with the definition $*$, the probability density is given in terms of the wavefunction by

$$\boxed{P(\vec{x}_1, \vec{x}_2) = 2\,|\psi_S(\vec{x}_1, \vec{x}_2)|^2.}$$

- all the above applies also to fermions:

$$|\vec{x}_1\vec{x}_2, A\rangle \doteq \frac{1}{\sqrt{2}}\left(|\vec{x}_1\vec{x}_2\rangle - |\vec{x}_2\vec{x}_1\rangle\right)$$

$$\langle x_1 x_2, A | y_1 y_2 A\rangle = \delta^3(x_1-y_1)\,\delta^3(x_2-y_2) - \delta^3(x_1-y_2)\,\delta^3(x_2-y_1)$$

$$1_A = \frac{1}{2}\int d^3x_1\, d^3x_2\, |x_1 x_2, A\rangle\langle x_1 x_2, A|$$

$$\psi_A(x_1 x_2) \doteq \frac{1}{\sqrt{2}}\langle x_1 x_2, A | \psi_A\rangle = -\psi_A(x_2, x_1).$$

- Examples

– Say 2 identical bosons are in the (normalized) single-particle states $|n_1\rangle$ & $|n_2\rangle$. Then the state of the 2 particles is

$$|\psi\rangle = \mathcal{N}\left(|n_1, n_2\rangle + |n_2, n_1\rangle\right).$$

What is $\mathcal{N}$? Determine it by the normalization condition:

$$1 = \langle\psi|\psi\rangle = |\mathcal{N}|^2 \left(\langle n_1, n_2| + \langle n_2, n_1|\right)\left(|n_1, n_2\rangle + |n_2, n_1\rangle\right)$$

$$= |\mathcal{N}|^2 \cdot 2\left(\cancelto{1}{\langle n_1|n_1\rangle} \cdot \cancelto{1}{\langle n_2|n_2\rangle} + \langle n_1|n_2\rangle\langle n_2|n_1\rangle\right)$$

$$\therefore\ \mathcal{N} = \frac{1}{\sqrt{2}} \cdot \frac{1}{\sqrt{1 + |\langle n_1|n_2\rangle|^2}}.$$

So $\mathcal{N} = \frac{1}{\sqrt{2}}$ only if $\langle n_1|n_2\rangle = 0$.

– Say $\langle n_1|n_2\rangle = 0$, so $\mathcal{N} = \frac{1}{\sqrt{2}}$. What is $\psi(x_1, x_2)$?

$$\psi(x_1, x_2) \doteq \frac{1}{\sqrt{2}}\langle x_1, x_2, S|\psi\rangle$$

$$= \frac{1}{\sqrt{2}} \cdot \frac{1}{\sqrt{2}}\left(\langle x_1, x_2| + \langle x_2, x_1|\right)\frac{1}{\sqrt{2}}\left(|n_1, n_2\rangle + |n_2, n_1\rangle\right)$$

$$= \frac{1}{2\sqrt{2}}\Big(\langle x_1|n_1\rangle\langle x_2|n_2\rangle + \langle x_1|n_2\rangle\langle x_2|n_1\rangle$$

$$+ \langle x_2|n_1\rangle\langle x_1|n_2\rangle + \langle x_2|n_2\rangle\langle x_1|n_1\rangle\Big)$$

$$= \frac{1}{\sqrt{2}}\Big(\langle x_1|n_1\rangle\langle x_2|n_2\rangle + \langle x_2|n_1\rangle\langle x_1|n_2\rangle\Big)$$

$$= \frac{1}{\sqrt{2}}\Big(\psi_{n_1}(x_1)\psi_{n_2}(x_2) + \psi_{n_2}(x_1)\psi_{n_1}(x_2)\Big)$$

"Symmetized product of wave functions"

- Say 2 ident. fermions in $|n_1\rangle, |n_2\rangle$ & $\langle n_1|n_2\rangle = 0$

Then $|\psi\rangle = \frac{1}{\sqrt{2}}\Big(|n_1, n_2\rangle - |n_2, n_1\rangle\Big)$ &

$$\psi(x_1 x_2) = \frac{1}{\sqrt{2}}\langle x_1 x_2, A|\psi\rangle$$

$$= \frac{1}{2\sqrt{2}}\Big(\langle x_1 x_2| - \langle x_2 x_1|\Big)\Big(|n_1 n_2\rangle - |n_2 n_1\rangle\Big)$$

$$= \frac{1}{2\sqrt{2}}\Big(\langle x_1|n_1\rangle\langle x_2|n_2\rangle - \langle x_1|n_2\rangle\langle x_2|n_1\rangle$$
$$- \langle x_2|n_1\rangle\langle x_1|n_2\rangle + \langle x_2|n_2\rangle\langle x_1|n_1\rangle\Big)$$

$$= \frac{1}{\sqrt{2}}\Big(\langle x_1|n_1\rangle\langle x_2|n_2\rangle - \langle x_1|n_2\rangle\langle x_2|n_1\rangle\Big)$$

$$= \frac{1}{\sqrt{2}}\det\begin{pmatrix}\langle x_1|n_1\rangle & \langle x_1|n_2\rangle \\ \langle x_2|n_1\rangle & \langle x_2|n_2\rangle\end{pmatrix}$$

"Slater determinant"

Statistics & probability distributions

Consider 2 particles in o-n states $|n\rangle, |m\rangle$. Then the 2-particle wave function is

$$\psi_D(x_1 x_2) = \psi_n(x_1)\psi_m(x_2) \qquad \text{distinguishable}$$

$$\psi_S(x_1 x_2) = \frac{1}{\sqrt{2}}\left(\psi_n(x_1)\psi_m(x_2) + \psi_m(x_1)\psi_n(x_2)\right) \qquad \text{boson}$$

$$\psi_A(x_1 x_2) = \frac{1}{\sqrt{2}}\left(\psi_n(x_1)\psi_m(x_2) - \psi_m(x_1)\psi_n(x_2)\right) \qquad \text{fermion}$$

Then probability density to find at $(\vec{x}_1, \vec{x}_2)$ is $|\psi|^2$:

$$P_D(x_1 x_2) = |\psi_n(x_1)|^2 \cdot |\psi_m^2(x_2)|$$

$$P_S(x_1 x_2) = 2|\psi_S(x_1 x_2)|^2 = |\psi_n(x_1)\psi_m(x_2) + \psi_n(x_2)\psi_m(x_1)|^2$$

$$= \left\{ |\psi_n(x_1)|^2 |\psi_m(x_2)|^2 + |\psi_m(x_1)|^2 \cdot |\psi_n(x_2)|^2 \right.$$
$$\left. + \left[\psi_n(x_1)\psi_m(x_2)\psi_m^*(x_1)\psi_n^*(x_2) + c.c.\right]\right\}$$

$$P_A(x_1 x_2) = 2|\psi_A(x_1 x_2)|^2 = |\psi_n(x_1)\psi_m(x_2) - \psi_n(x_2)\psi_m(x_1)|^2$$

$$= \left\{ |\psi_n(x_1)|^2 |\psi_m(x_2)|^2 + |\psi_m(x_1)|^2 \cdot |\psi_n(x_2)|^2 \right.$$

$$- \left[\psi_n(x_1)\psi_m(x_2)\psi_m^*(x_1)\psi_n^*(x_2) + c.c. \right] \Big\}$$

$\therefore$ Different probability distributions.

- E.g., say state $|n\rangle$ is localized near x_1
  and " $|m\rangle$ " " " x_2

  i.e. $\psi_n(x_1) \neq 0$, $\psi_m(x_2) \neq 0$
  & $\psi_n(x_2) = 0$, $\psi_m(x_1) = 0$

  Then $P_S(x_1,x_2) = P_A(x_1,x_2) = P_D(x_1,x_2)$.

- E.g. say $x_1 = x_2 \doteq x$ (& $\psi_n(x) \neq 0$ & $\psi_m(x) \neq 0$)

$$P_D(x,x) = |\psi_n(x)|^2 |\psi_m(x)|^2$$

$$P_S(x,x) = 4\,|\psi_n(x)|^2 |\psi_m(x)|^2 = 4\,P_D(x,x)$$ "statistical attraction"

$$P_A(x,x) = 0$$ "statistical repulsion"

2 identical particles $\to$ N identical particles

- $N=3$

$$|a_1, a_2, a_3; S/A\rangle \doteq$$

$$\frac{1}{\sqrt{3!}}\Big\{\big(|a_1 a_2 a_3\rangle + |a_3 a_1 a_2\rangle + |a_2 a_3 a_1\rangle\big) \pm \big(|a_3 a_2 a_1\rangle + |a_1 a_3 a_2\rangle + |a_2 a_1 a_3\rangle\big)\Big\}$$

Note: correct normalization factor only if $|a_1\rangle \neq |a_2\rangle \neq |a_3\rangle$ & are all orthonormal.

$+$ = completely symmetrized
$-$ = completely antisymmetrized

$$1_{S/A} = \frac{1}{3!}\int dx_1 dx_2 dx_3\, |x_1 x_2 x_3, S/A\rangle\langle x_1 x_2 x_3, S/A|$$

$$\psi_{S/A}(x_1 x_2 x_3) \doteq \frac{1}{\sqrt{3!}}\langle x_1 x_2 x_3, S/A|\psi_{S/A}\rangle$$

$$= \frac{1}{3!}\Big\{\big(\langle x_1 x_2 x_3| + \langle x_3 x_1 x_2| + \langle x_2 x_3 x_1|\big) \pm \big(\langle x_3 x_2 x_1| + \langle x_1 x_3 x_2| + \langle x_2 x_1 x_3|\big)\Big\}|\psi_{S/A}\rangle$$

$$= \langle x_1 x_2 x_3 | \Psi_{S/A} \rangle$$

$$\Rightarrow \quad 1 = \langle \Psi_{S/A} | \Psi_{S/A} \rangle = \cdots = \int dx_1 dx_2 dx_3 \, |\Psi_{S/A}(x_1 x_2 x_3)|^2$$

& $$P(x_1 x_2 x_3) = (3!) \, |\Psi_{S/A}(x_1 x_2 x_3)|^2$$

& $$\Psi_{a_1 a_2 a_3 S/A}(x_1 x_2 x_3) = \frac{1}{\sqrt{3!}} \Big(\psi_{a_1}(x_1) \psi_{a_2}(x_2) \psi_{a_3}(x_3) \pm \underset{\text{of } (a_1 a_2 a_3)}{\overset{5 \text{ more}}{\text{permutations}}} \Big)$$

& $$\Psi_{a_1 a_2 a_3 A} = \frac{1}{\sqrt{3!}} \det \begin{pmatrix} \psi_{a_1}(x_1) & \psi_{a_1}(x_2) & \psi_{a_1}(x_3) \\ \psi_{a_2}(x_1) & \psi_{a_2}(x_2) & \psi_{a_2}(x_3) \\ \psi_{a_3}(x_1) & \psi_{a_3}(x_2) & \psi_{a_3}(x_3) \end{pmatrix} .$$

- Note, however, that

$$V^{\otimes 3} \doteq V \otimes V \otimes V$$

$$\neq V_S \oplus V_A \quad , \quad b/c$$

$$\text{dim:} \quad n^3 \neq \frac{n(n+1)(n+2)}{3!} + \frac{n(n-1)(n-2)}{3!} \underset{n \gg 1}{\approx} \frac{n^3}{3}$$

For 3 or more particles, there are more possibilities for states than total symmetrization or total antisymmetrization.

- Larger N:

- Say $\{|a\rangle, a=1\cdots n\}$ is ON basis of V

- Then $\frac{1}{\sqrt{N!}}\sum_{\pi\in S_N}(\pm)^{\pi}|a_{\pi(1)}a_{\pi(2)}\cdots a_{\pi(N)}\rangle \in V_{S/A}$

where: $S_N \doteq$ group of permutations on N objects ("symmetric group")

$$N! = |S_N|$$

$$\pi\in S_N : (123\cdots N) \mapsto (\pi(1)\,\pi(2)\cdots\pi(N))$$

$(-)^{\pi} \doteq$ sign of permutation π
$= (-)^{\#\text{ of pairwise interchanges needed to arrive at }\pi}$.

- $\dim V_S = \binom{n+N-1}{N} \doteq \frac{(n+N-1)!}{N!(n-1)!}$

- $\dim V_A = \binom{n}{N} \doteq \frac{n!}{N!(n-N)!}$ $(\doteq 0$ if $n<N)$

$n \doteq$ dim 1-particle Hilbert space

$N \doteq$ number of particles

- Beginning of whole formalism ...

Spin & statistics

- Special relativity + quantum mechanics (+ locality) implies the

$$\boxed{\begin{array}{c}\text{Spin-Statistics theorem:}\\ \text{Identical integer-spin particles are bosons, \&}\\ \text{identical half-odd-integer-spin particles are fermions}\end{array}}$$

- E.g.: e^-, p, n have $s = 1/2$ $\Rightarrow$ fermions

  & : $\pi^\pm$, γ, $H_{(n=1)}$ have $s = 0, 1, 0 \text{ or } 1$, resp. $\Rightarrow$ bosons.

  ground state of H-atom.

- The "spin" of a composite object, like $H_{(n=1)}$ is just its total angular momentum.

$$H_{n=1} = \underset{(s=1/2)}{e^-} + \underset{(s=1/2)}{p} \quad \text{in an } \ell = 0 \text{ state.}$$

Recall "addition of angular momentum" from fall : " $\frac{1}{2} \otimes \frac{1}{2} = 0 \oplus 1$ " :

$$\vec{J} = \vec{S}_{e^-} + \vec{S}_p + \vec{L}$$

$$V_{s=1/2} \otimes V_{s=1/2} \otimes V_{\ell=0} = V_{j=0} \oplus V_{j=1}$$

$$\text{dim} = \quad 2 \quad \times \quad 2 \quad \times \quad 1 \quad = \quad 1 \quad + \quad 3$$

So total ang. mom. of $H_{(n=1)}$ can be either $j=0$ or $j=1$, depending on spin states of e^- & p. So we say $H_{(n=1)}$ has spin 0 or 1. In either case, it is a boson.

- In general any collection of b bosons + f fermions with spins $(s_i \;\; i=1\ldots b)$ + $(\hat{s}_j \;\; j=1\ldots f)$ will have total spin

$$\vec{J} = \sum_{i=1}^{b} \vec{S}_i + \sum_{j=1}^{f} \vec{\hat{S}}_j + \vec{L}$$

acting on Hilbert space

$$V_{tot} = V_{s_1} \otimes \cdots \otimes V_{s_b} \otimes V_{\hat{s}_1} \otimes \cdots \otimes V_{\hat{s}_f} \otimes V_{\ell}$$

Repeated use of the addition of angular momentum formula

$$V_{j_1} \otimes V_{j_2} = V_{|j_1-j_2|} \oplus V_{|j_1-j_2|+1} \oplus \cdots \oplus V_{j_1+j_2}$$

implies

$$V_{tot} = \bigoplus_j V_j$$

with $$j = \sum_{i=1}^{b} s_i + \sum_{j=1}^{f} \hat{s}_j + l - n$$

for some integers $n \in \mathbb{Z}$. But $l \in \mathbb{Z}$, $s_i \in \mathbb{Z}$, $\hat{s}_j \in \mathbb{Z} + \frac{1}{2}$, so

$$j \in \begin{cases} \mathbb{Z} & \text{if } f \text{ is even} \\ \mathbb{Z}+\frac{1}{2} & \text{" " odd.} \end{cases}$$

Any boundstate of b bosons + f fermions has integer spin if f is even and half-odd-integer spin if f is odd.

$\therefore$ Spin-statistics $\Rightarrow$ bound state is a boson if f is even and a fermion if f is odd.

See problem set for argument just from (anti)symmetry of wave function that this must be true.

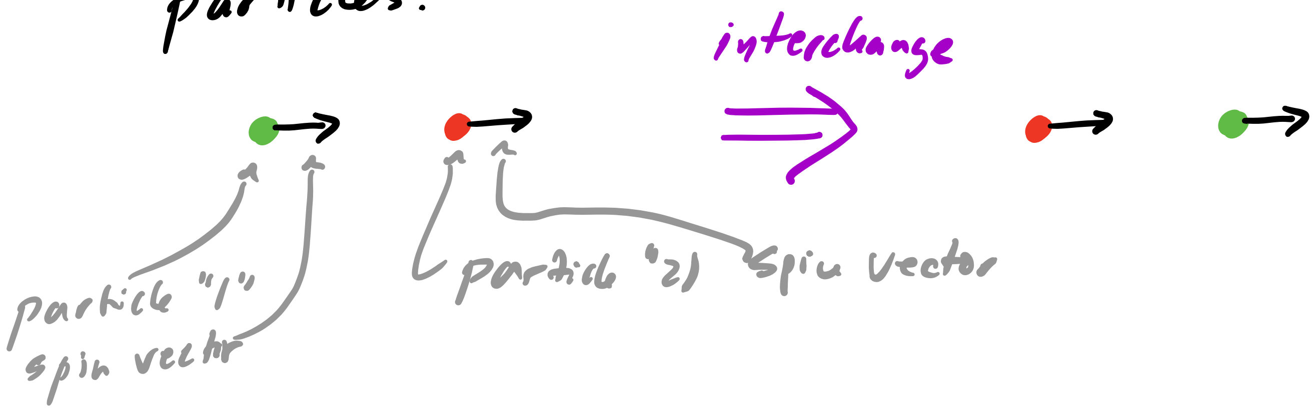
- Intuitive argument for the spin-statistics theorem:

Interchanging 2 identical particles in space is equivalent to rotating one of them by 2π relative to the other. But a 2π-rotation operator

$$R(2\pi) = \begin{cases} +1 & \text{for } s \in \mathbb{Z} \\ -1 & \text{for } s \in \mathbb{Z} + \frac{1}{2}. \end{cases}$$

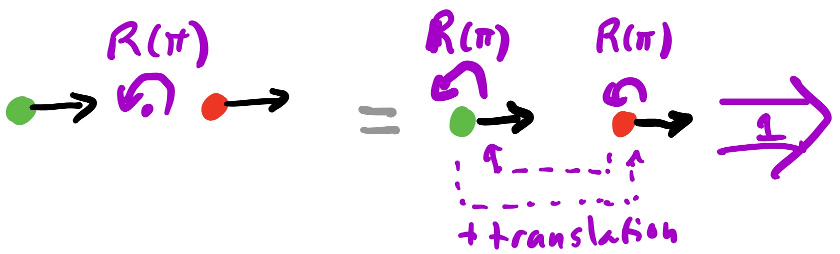
So interchanging 2 identical $s \in \mathbb{Z}$ particles gives a $(+1)$ phase in the state, and a (-1) phase for $s \in \mathbb{Z} + \frac{1}{2}$ particles. ✓

- More detail: interchange 2 identical particles:



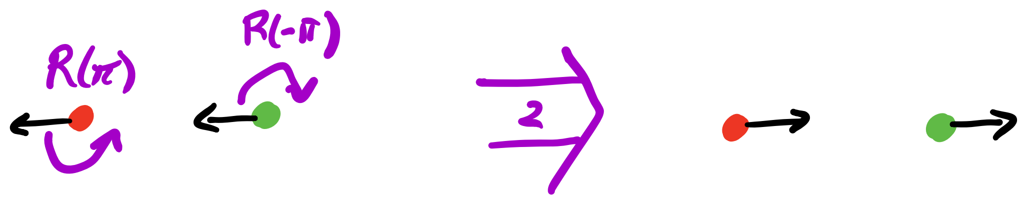
as follows.

Step 1 Rotate by π counterclockwise $= R(\pi)$

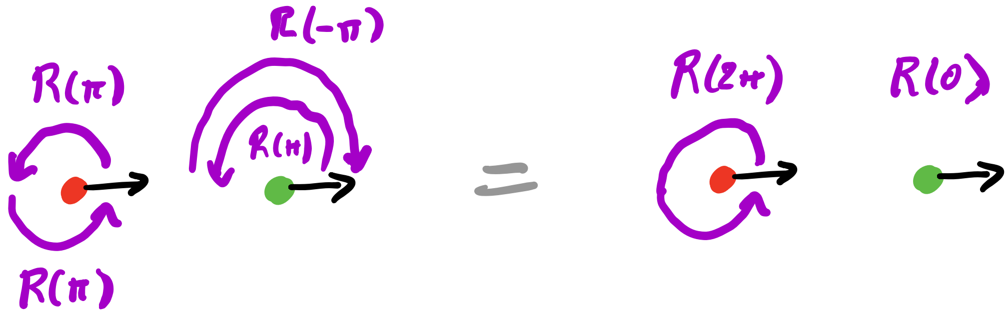


ARGUMENT?

Step 2 Rotate 



So net affect on spins is:



NOT REALLY A CONVINCING

$$\text{Now } \hat{R}(0) = e^{0\cdot i\hat{J}_z/\hbar} = e^0 = \hat{1}, \text{ but}$$

$$\hat{R}(2\pi) = e^{2\pi i\hat{J}_z/\hbar} = \exp\left\{2\pi i\begin{pmatrix} s & & & \\ & s-1 & & \\ & & \ddots & \\ & & & 1-s & \\ & & & & -s\end{pmatrix}\right\}$$

$$= \begin{pmatrix} e^{2\pi i s} & & & & \\ & e^{2\pi i(s-1)} & & & \\ & & \ddots & & \\ & & & e^{2\pi i(1-s)} & \\ & & & & e^{2\pi i(-s)}\end{pmatrix} = e^{2\pi i s}\begin{pmatrix} 1 & & & & \\ & 1 & & & \\ & & \ddots & & \\ & & & 1 & \\ & & & & 1\end{pmatrix} = e^{2\pi i s}\cdot\hat{1}$$

Since $e^{2\pi i s} = \begin{cases} +1 & s\in\mathbb{Z} \\ -1 & s\in\mathbb{Z}+\frac{1}{2}\end{cases}$, therefore

$$\hat{R}(2\pi) = \begin{cases} +\hat{1} & s\in\mathbb{Z} \\ -\hat{1} & s\in\mathbb{Z}+\frac{1}{2}.\end{cases}$$

Some implications of spin & statistics

- spin-1/2 particles (e.g. electrons)

  - If the electrons had only spin states $\{|\pm\rangle\} \doteq V_{j=1/2}$, then antisymmetry would imply that they could only be in the state

$$|\psi\rangle = \frac{1}{\sqrt{2}}\left(|+-\rangle - |-+\rangle\right).$$

  - Recall addition of angular momentum

$$\underset{\{|\pm\rangle\} \otimes \{|\pm\rangle\}}{V_{j=1/2} \otimes V_{j=1/2}} = \underbrace{V_{j=0} \oplus V_{j=1}}_{|j,m\rangle}.$$

with $|j,m\rangle =$

$$|0,0\rangle = \frac{1}{\sqrt{2}}\left(|+-\rangle - |-+\rangle\right) \quad \Big\} \; V_{j=0} = V_A$$

$$\left.\begin{aligned} |1,1\rangle &= |++\rangle \\ |1,0\rangle &= \frac{1}{\sqrt{2}}\left(|+-\rangle + |-+\rangle\right) \\ |1,-1\rangle &= |--\rangle \end{aligned}\right\} \; V_{j=1} = V_S$$

- But particles also have position/momentum degrees of freedom.
  - For example, an electron in a hydrogen atom energy eigenstate is described by $|nlm\rangle$. Adding in spin, get o-n basis of states

$$|nlm, m_s\rangle = |nlm, \pm\rangle$$

$\pm \frac{1}{2}$ $\hat{S}_z/\hbar$ eigenvalues.

- So 2 e^-'s in the same H-atom potential will have a basis of states

$$|n_1 l_1 m_1, \pm\rangle \otimes_A |n_2 l_2 m_2, \pm\rangle$$

(means: antisymmetric combo.) ...

- Let's practice antisymmetrizing on multiple quantum numbers with a simpler example.

Say e^- Hilb. space has basis $\{|a\rangle, |b\rangle\}$.

Then general $2e^-$ states are

$$|a_1 b_1\rangle \otimes_A |a_2 b_2\rangle$$

$$\doteq \frac{1}{\sqrt{2}}\left(|a_1 b_1\rangle |a_2 b_2\rangle - |a_2 b_2\rangle |a_1 b_1\rangle\right)$$

$$\doteq \frac{1}{\sqrt{2}}\left(|a_1 a_2\rangle \otimes |b_1 b_2\rangle - |a_2 a_1\rangle \otimes |b_2 b_1\rangle\right)$$

where I have re-ordered tensor-product basis from $(V_a)_1 \otimes (V_b)_1 \otimes (V_a)_2 \otimes (V_b)_2 \to (V_a)_1 \otimes (V_a)_2 \otimes (V_b)_1 \otimes (V_b)_2$.

Then

$$\boxed{|a_1 b_1\rangle \otimes_A |a_2 b_2\rangle} =$$

$$\begin{aligned}
= \frac{1}{\sqrt{2}} \Big\{ & \tfrac{1}{2}\left(|a_1 a_2\rangle + |a_2 a_1\rangle\right) \otimes |b_1 b_2\rangle \\
& + \tfrac{1}{2}\left(|a_1 a_2\rangle - |a_2 a_1\rangle\right) \otimes |b_1 b_2\rangle \\
& - \tfrac{1}{2}\left(|a_1 a_2\rangle + |a_2 a_1\rangle\right) \otimes |b_2 b_1\rangle \\
& + \tfrac{1}{2}\left(|a_1 a_2\rangle - |a_2 a_1\rangle\right) \otimes |b_2 b_1\rangle \Big\}
\end{aligned}$$

$$\begin{aligned}
= \frac{1}{\sqrt{2}} \Big\{ & \tfrac{1}{2}\left(|a_1 a_2\rangle + |a_2 a_1\rangle\right) \otimes \left(|b_1 b_2\rangle - |b_2 b_1\rangle\right) \\
& + \tfrac{1}{2}\left(|a_1 a_2\rangle - |a_2 a_1\rangle\right) \otimes \left(|b_1 b_2\rangle + |b_2 b_1\rangle\right) \Big\}
\end{aligned}$$

$$\boxed{= \frac{1}{\sqrt{2}}\left(|a_1 a_2, S\rangle \otimes |b_1 b_2, A\rangle + |a_1 a_2, A\rangle \otimes |b_1 b_2, S\rangle\right)}$$

- Similarly for bosons:

$$\boxed{\begin{aligned}&|a_1 b_1\rangle \otimes_S |a_2 b_2\rangle = \\ &= \tfrac{1}{\sqrt{2}}\Big(|a_1 a_2, S\rangle \otimes |b_1 b_2, S\rangle + |a_1 a_2, A\rangle \otimes |b_1 b_2, A\rangle\Big)\end{aligned}}$$

- For 2 e^-'s: if a's = orbital qu. no's & b's = spin quantum numbers, then 2-e^- state will be

$$\frac{1}{\sqrt{2}}\Big(|a_1 a_2, S\rangle \otimes \underbrace{|b_1 b_2, A\rangle}_{|j=0\rangle} + |a_1 a_2, A) \otimes |\underbrace{b_1 b_2, S}_{|j=1, m\rangle}\rangle\Big)$$

- Examples

- Say 2 e^-'s in orbital ground state $|n\ell m\rangle = |100\rangle$ of H-atom. Then

$$|\psi\rangle = |(100)_1 (100)_2, S\rangle \otimes \frac{1}{\sqrt{2}}\big(|+-\rangle - |-+\rangle\big)$$

$$= |100\rangle_1 |100\rangle_2 \otimes |j=0\rangle_A$$

since $|(100)_1 (100)_2, A\rangle \equiv 0$.

- But if both in $n=2, l=1$ orbital states
$|n l m\rangle = |2 1 m\rangle \quad m \in \{-1,0,1\}$
then can be any of the states

$\{ |21 m, m_s\rangle \}$ $3\cdot 2 = 6$ states, so
$|21 m, m_s\rangle \otimes_A |21 m', m_s'\rangle = \frac{6\cdot 5}{2} = 15$ states

which can be written in basis

$|(21m_1)(21m_2); S\rangle \otimes |j=0\rangle_A \; \Big\} \; \frac{3\cdot 4}{2} = 6$ states
& $\qquad\qquad\qquad\qquad +$
$|(21m_1)(21m_2); A\rangle \otimes |j=1, m_j\rangle_S \; \Big\} \; \frac{3\cdot 2}{2}\cdot 3 = 9$ states

15 states ✓

- Total angular momentum

$$\underset{\substack{\uparrow \\ l=1}}{|\,2\,1}\; m, \underset{\substack{\uparrow \\ s=1/2}}{m_s}\rangle : \quad \underset{3}{(l=1)} \otimes \underset{2}{(s=1/2)} = \underset{2}{(j=\tfrac{1}{2})} \oplus \underset{4}{(j=\tfrac{3}{2})}$$
$$3 \cdot 2 = 2 + 4$$

$\{ |21 m, m_s\rangle \otimes_A |21 m', m_s'\rangle \}$:

$$\big[\overset{2}{(j=\tfrac{1}{2})} \overset{+}{\oplus} \overset{4}{(j=\tfrac{3}{2})}\big] \otimes_A \big[\overset{2}{(j=\tfrac{1}{2})} \overset{+}{\oplus} \overset{4}{(j=\tfrac{3}{2})}\big] \quad = \frac{6\cdot 5}{2} = 15$$

$$= \underbrace{\big[\underset{2}{(j=\tfrac{1}{2})} \overset{\cdot}{\otimes_A} \underset{2}{(j=\tfrac{1}{2})}\big]}_{2\cdot 1/2 = 1} \oplus \big[\underset{2}{(j=\tfrac{1}{2})} \overset{\cdot}{\otimes} \underset{4}{(j=\tfrac{3}{2})}\big] = 8$$
$$\oplus \big[(j=3/2) \otimes_A (j=3/2)\big]$$

$$= \underset{1}{(j=0)} \oplus \Big[\underset{3}{(j=1)} \underset{+}{\oplus} \underset{5}{(j=2)}\Big]$$

$$\underbrace{4 \cdot 4}_{4\cdot 3/2 = 6}$$

$$\oplus \Big[\underset{1}{(j=0)} \underset{A\ +}{\oplus} \underset{3}{\cancel{(j=1)}} \underset{+}{\oplus} \underset{5}{(j=2)} \underset{A\ +}{\oplus} \underset{7}{\cancel{(j=3)}}\Big]$$

$\therefore$ 2 e^-'s in $n=2$, $\ell=1$ orbital live in a $6\cdot 5/2 = 15$-dim'l Hilbert space which can be decomposed into $\hat{J}^2$ eigenspaces

"$j = 0 \oplus 0 \oplus 1 \oplus 2 \oplus 2$"

of dim $1 + 1 + 3 + 5 + 5 = 15$ ✓

Multi-electron atoms

- Simplest: Helium

  Nucleus has $Z=2$, i.e. charge $+2e$ & 2 e^-'s, each of charge $-e$, so Hamiltonian (for relative motion) is

$$\hat{H}_{He} = \underbrace{\left(\frac{\hat{P}_1^2}{2\mu} - \frac{2e^2}{\hat{r}_1}\right) + \left(\frac{\hat{P}_2^2}{2\mu} - \frac{2e^2}{\hat{r}_2}\right)}_{\substack{\text{2 copies of } Z=2 \text{ hydrogenic atom} \\ \doteq \hat{H}_0}} + \underbrace{\frac{e^2}{|\vec{r}_1 - \vec{r}_2|}}_{\substack{e\text{-}e \text{ interaction} \\ \doteq \hat{H}_1}}$$

$\therefore \quad \hat{H}_{He} = \hat{H}_0 + \hat{H}_1$

- If ignore $\hat{H}_1$ (say, it is $\ll \hat{H}_0$) then ground state of $\hat{H}_0$ is

$$|n=1\rangle_{He} = |(100)_1 (100)_2\rangle_S \otimes |j=0\rangle_A$$

w/ $j_{tot} = 0$ ✓ , $E_{He} = 2 \cdot Z^2 \cdot E_H = 8 \cdot E_H$. ✗

($\approx 5.8\, E_H$ experimentally)

- Treat $\hat{H}_1$ as perturbation, find 1st-order pert. theory gives an answer within 10% of experimental value. (But then 2nd order gives worse...) (See pp. 424-428 Townsend)

- No reason to expect p.t. to work:

$$\frac{e^2}{|r_1 - r_2|} \approx \frac{e^2}{a_0} \approx \text{same order of magnitude}$$

as terms in $\hat{H}_0$!

- Another approach which gives a better approximation to E_{He} is the

Variational Method.

- Say $\{ |E_n\rangle \;\; n=1,2,\cdots \}$ is o-n exact energy eigenbasis of $\hat{H}_{He}$, ordered so that $E_1 \leq E_2 \leq E_3 \leq \cdots$.

  Then <u>any</u> state $|\psi\rangle$ can be written

$$|\psi\rangle = \sum_{n=1}^{\infty} c_n |E_n\rangle \; . \quad \left(\sum_n |c_n|^2 = 1 \right)$$

  Compute

$$\langle\psi|\hat{H}_{He}|\psi\rangle = \sum_{n,m=1}^{\infty} c_m^* c_n \langle E_m|\hat{H}_{He}|E_n\rangle$$

$$= \sum_{n,m=1}^{\infty} c_m^* c_n E_n \delta_{m,n} = \sum_{n=1}^{\infty} |c_n|^2 E_n$$

$$\geq E_1 \cdot \left(\sum_{n=1}^{\infty} |c_n|^2 \right) = E_1$$

$$\therefore \quad \boxed{\langle\psi|\hat{H}_{He}|\psi\rangle \geq E_1}$$

- Variational method: ① choose a <u>family</u> of "trial ground states" (i.e., guesses)

$$|\psi(\alpha)\rangle$$

where α are some adjustable parameters.

② Compute

$$E(\alpha) \doteq \langle \Psi(\alpha) | \hat{H}_{He} | \Psi(\alpha) \rangle.$$

③ Minimize $E(\alpha)$, i.e., solve for α_* such that

$$\left.\frac{dE(\alpha)}{d\alpha}\right|_{\alpha=\alpha_*} = 0 \quad \text{\& minimum.}$$

Then $E(\alpha_*) \geq E_{He}$ is new estimate.

- Clearly depends on guess of $|\Psi(\alpha)\rangle$.

E.g., if choose

$$\langle \vec{x}_1, \vec{x}_2 | \Psi(\alpha) \rangle = \frac{Z^3}{\pi a^3} e^{-Z(r_1+r_2)/a}, \quad \alpha \doteq (a, Z)$$

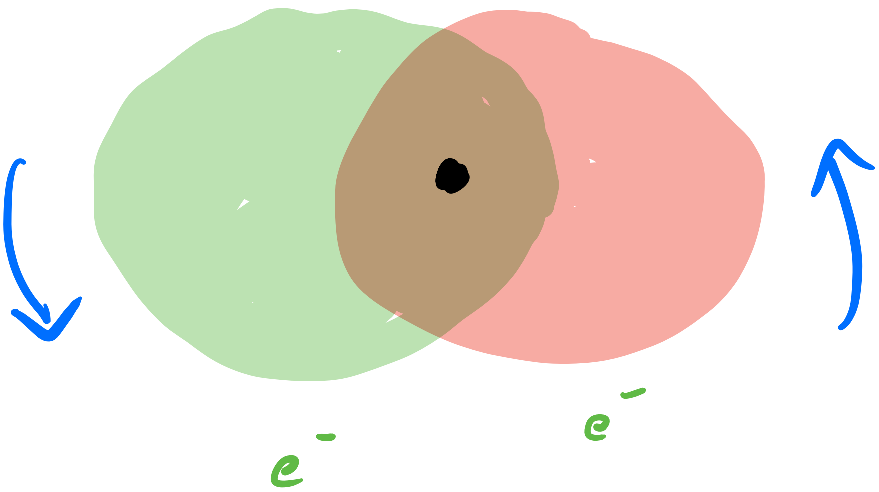
(& in $|j=0\rangle_A$ spin-singlet state)

then minimizing w.r.t. a, Z gives

$$E(\alpha^*) = \frac{1}{2}\left(\frac{3}{2}\right)^6 E_H \approx 5.7\, E_H$$

which is accurate to < 2%.

- But does this really tell us anything beyond a better upper bound on the energy? The variational wavefunction was involved no correlation between the two electrons, whereas expect them to repel one-another



- Nevertheless, ignoring the e-e interaction gives a qualitatively very good picture of the spins & ionization energies of atomic ground states, reproducing much of the periodic table ... See §12.3 Townsend.
- Famous example: metals & Fermi liquids ...