

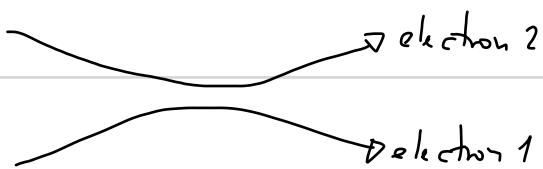
## Identical particles [CT XIV / G ch.5]

Q: what happens when we have two physical objects, that are absolutely identical in all respects?

This is a weird question - and from the point of view of classical physics, ultimately a meaningless one, for it is not clear such a thing can even exist!

Two macroscopic objects are clearly never entirely identical - there is always some small enough difference. What about 2 point particles?

Consider a system of two particles who share all the same internal attributes (same mass, charge, etc). Even if they are internally identical, we can always tell which is which in principle, however, as long as we follow their trajectories over time → even if they interact, or collide.



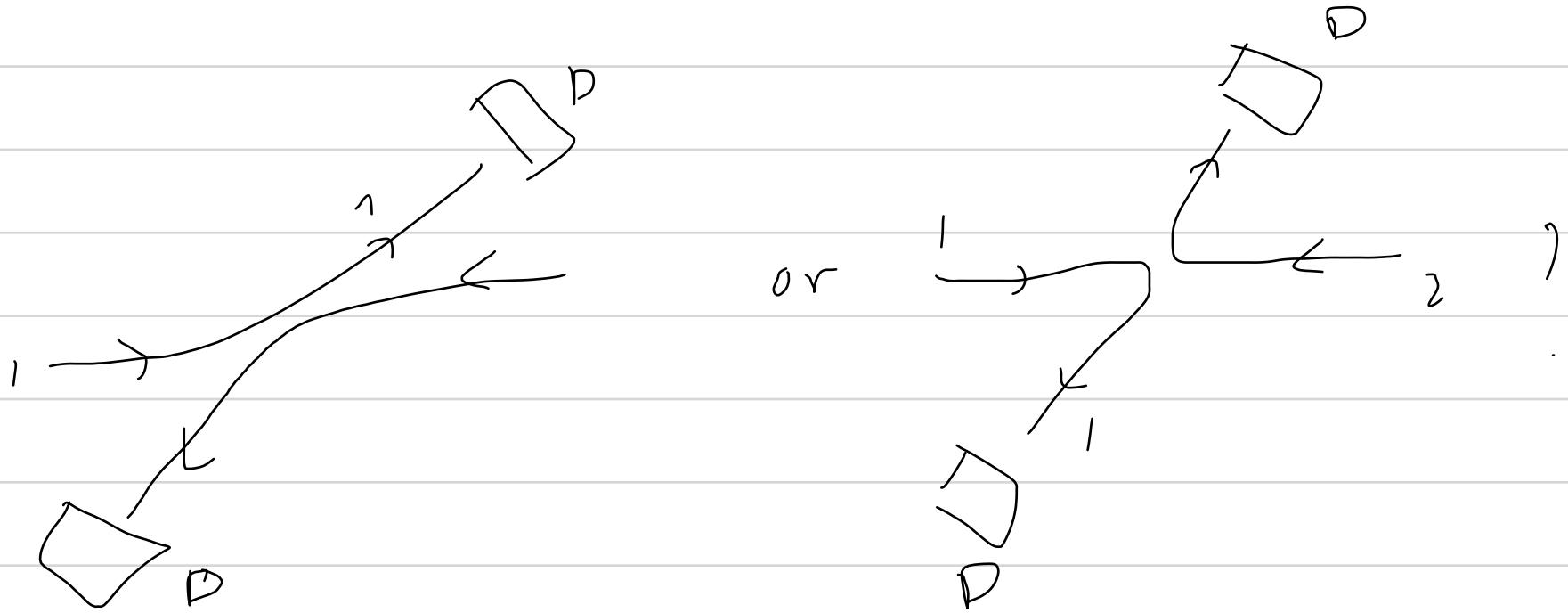
The fact that both particles are 'of the same type' is however reflected in our dynamical description of this 2 particle system: its classical Hamiltonian (or Lagrangian, f.ex.) must retain the same form if we exchange the label used to refer to each particle (we say it is "invariant under permutation" of the particles)

Ex:  $H = H_1 + H_2 + H_{int}$ , where either  $H_j$  is the same function, but calculated on different variables  $r_j, p_j, t$ , and  $H_{int}$  is some function of  $r_1, r_2, p_1, p_2, t$ , such that  

$$H_{int}(r_1, r_2, p_1, p_2, t) = H_{int}(r_2, r_1, p_2, p_1, t) \quad )$$

In QM however, the situation is different, because particles don't have trajectories, only wavefunctions, and 2 different particles can in fact have overlapping wf's! Furthermore, we don't measure a particle's position at each instant, only its amplitude for moving from initial position (or state)  $|\psi_i\rangle$  to a final one  $|\psi_f\rangle$  after some time  $t$

$$\langle \psi_f | U_{\text{evol}}(t) | \psi_i \rangle$$



- problem posed by lack of trajectories: more than one description compatible
  - in collisions: what is the final state  $|\psi_1\rangle_A |\psi_2\rangle_B$  or  $|\psi_2\rangle_A |\psi_1\rangle_B$  ?

- same problem w initial states:

states of the form  $\alpha|+-\rangle + \beta|+-\rangle$  lead to different predictions for  $P(S_{X_A}=S_{X_B}=+)$

$$\text{ex: } \left| \langle +_x +_x | (\alpha|+-\rangle + \beta|-+\rangle) \right|^2 = \left| \frac{1}{2}(\alpha + \beta) \right|^2$$

even more specifically: recall that states  $\frac{1}{\sqrt{2}}[|+-\rangle \pm |--\rangle]$  have very different ang. momentum!

→ we need some rule to specify which combination of  $\alpha, \beta$  to use

- Problem only gets worse w/ 3 or more particles : ex: 3 particles in states  $a, b, c \dots$

$$|abc\rangle, |acb\rangle, \dots$$

- principle : exchange of particles should leave physical predictions unchanged

[strangely: this argument is not pursued by CT]

consider  $|\psi\rangle = \sum_{ij} c_{ij} |e_i\rangle_A |e_j\rangle_B$  and  $|\tilde{\psi}\rangle = \sum_{ij} c_{ij} |e_j\rangle_A |e_i\rangle_B$  (ie:  $\tilde{c}_{ij} = c_{ji}$ )

In order to give all the same physical predictions, it must be true that  $|\tilde{\psi}\rangle = e^{i\theta} |\psi\rangle$   
for some global phase  $\theta$

In fact, in most situations it turns out that only 2 values for this phase occur:  $e^{i\theta} = \pm 1$

- why to understand this: exchanging the particles a second time makes them return to their initial conditions. Since this is (apparently at least) equivalent to not having ever exchanged them at all, then we expect that  $(e^{i\theta})^2 = 1 \rightarrow e^{i\theta} = \pm 1$ .

if  $f = 1$  :  $c_{ij} = c_{ji} \rightarrow$  state is symmetric under exchange of 2 identical particles  
 $f = -1$        $c_{ij} = -c_{ji} \rightarrow$  "      " antisymmetric "      "      "      "      "

In Nature, both kinds of symmetry exist: particles who only accept symmetric states are called bosons, and those who only accept antisymmetric are called fermions.

Example if  $|\psi\rangle_1, |\psi\rangle_2$  are 2 single-particle states

$$|\Psi_S\rangle_S \equiv N_S [|\psi\rangle_1|\psi\rangle_2 + |\psi\rangle_2|\psi\rangle_1] \text{ is a possible state for two bosons}$$

$$|\Psi_A\rangle_A \equiv N_A [|\psi\rangle_1|\psi\rangle_2 - |\psi\rangle_2|\psi\rangle_1] \text{ is a possible state for two fermions}$$

normalization factors       $N_A^{-1} \left[ 2 \pm 2\langle \psi | \psi \rangle \langle \psi | \psi \rangle \right] = 1 \rightarrow N_A^{-1} = \sqrt{2(1 \pm |\langle \psi | \psi \rangle|^2)}$

(in particular  $N_S = N_A = \sqrt{2}$  if  $\langle \psi | \psi \rangle = 0$ )

Note: this symmetry/antisymmetry property applies to the entire state, including both position and spin variables.

Note: there are some special situations where exchanging two objects twice is not equivalent to doing nothing - think of 2 strings braiding around each other. It turns out that in QM there are situations where analogous braiding effects occur, and where other solutions for the phase  $e^{i\theta}$  are possible. The 'particles' obeying these special rules are called 'anyons', since they can have 'any' phase. We won't discuss these here.)

### Spin-statistics connection

Experimental observation:  $\begin{cases} \text{all known bosons turn out to have } \underline{\text{integer}} \text{ spin} \\ \text{all known fermions have half-integer spin} \end{cases}$

ex: electrons, protons, neutrons (all spin  $1/2$ ) are fermions

ex: W and Z particles (force carriers of the weak force, spin 1) and the Higgs particle (spin 0) are bosons.

This relationship has no explanation in nonrelativistic QM, but can be derived (under certain quite general assumptions) in QFT: this is the famous "spin-statistics theorem"

### Important observation:

If we try to choose  $|\psi\rangle = |\varphi\rangle$  above, the antisym state  $|\psi\varphi\rangle_A$  vanishes!

$\Rightarrow$  Fermions obey the "Pauli exclusion principle":

Two identical fermions cannot occupy the same single-particle quantum state

Example if  $\Psi(\vec{r})$ ,  $\psi(\vec{r})$  are 2 orthogonal single-particle wavefunctions

$$\underbrace{\Psi(\vec{r}_1)\Psi(\vec{r}_2)}_{\text{symm wf}} \otimes \underbrace{\uparrow_1 \uparrow_2}_{\text{symm spin state}}$$

$$\underbrace{\frac{1}{\sqrt{2}} [\Psi(\vec{r}_1)\Psi(\vec{r}_2) + \Psi(\vec{r}_1)\Psi(\vec{r}_2)]}_{\text{symmetric wf}} \otimes \underbrace{\frac{1}{\sqrt{2}} (\uparrow_1 \downarrow_2 + \downarrow_1 \uparrow_2)}_{\text{symm. spin state}}$$

$$\underbrace{\frac{1}{\sqrt{2}} [\Psi(\vec{r}_1)\Psi(\vec{r}_2) - \Psi(\vec{r}_1)\Psi(\vec{r}_2)]}_{\text{antisymmetric wf}} \otimes \underbrace{\frac{1}{\sqrt{2}} (\uparrow_1 \downarrow_2 - \downarrow_1 \uparrow_2)}_{\text{antisym spin state}}$$

$$\underbrace{\frac{1}{\sqrt{2}} [\Psi(\vec{r}_1)\Psi(\vec{r}_2) \otimes \uparrow_1 \downarrow_2 + \Psi(\vec{r}_1)\Psi(\vec{r}_2) \otimes \downarrow_1 \uparrow_2]}_{\text{symmetric state entangled in position+spin}}$$

} all are possible states of two bosons  
(note: here the spin states  $\uparrow, \downarrow$  mean  $m = \pm \frac{\hbar}{2}$ )

$$\underbrace{\frac{1}{\sqrt{2}} [\Psi(\vec{r}_1)\Psi(\vec{r}_2) - \Psi(\vec{r}_1)\Psi(\vec{r}_2)]}_{\text{antisymmetric wf}} \otimes \underbrace{\uparrow_1 \uparrow_2}_{\text{symm. spin state}} \xrightarrow{\quad \quad \quad} \text{note here both fermions have the same spin state (this is ok)}$$

$$\underbrace{\frac{1}{\sqrt{2}} [\Psi(\vec{r}_1)\Psi(\vec{r}_2) + \Psi(\vec{r}_1)\Psi(\vec{r}_2)]}_{\text{symmetric wf}} \otimes \underbrace{\frac{1}{\sqrt{2}} (\uparrow_1 \downarrow_2 - \downarrow_1 \uparrow_2)}_{\text{antisym spin state}}$$

} all are possible states of two fermions  
(note: here the spin states  $\uparrow, \downarrow$  mean  $m = \pm \frac{\hbar}{2}$ )

$$\underbrace{\Psi(\vec{r}_1)\Psi(\vec{r}_2)}_{\text{symmetric wf}} \otimes \underbrace{\frac{1}{\sqrt{2}} (\uparrow_1 \downarrow_2 - \downarrow_1 \uparrow_2)}_{\text{antisym spin state}}$$

$$\underbrace{\frac{1}{\sqrt{2}} [\Psi(\vec{r}_1)\Psi(\vec{r}_2) \otimes \uparrow_1 \downarrow_2 - \Psi(\vec{r}_1)\Psi(\vec{r}_2) \otimes \downarrow_1 \uparrow_2]}_{\text{anti-symmetric state entangled in position+spin}}$$

Note: these are just useful examples, not the most general possibilities!

## Consequences

i) bosons, fermions and distinguishable particles have very different properties (e.g. energy eigenstates/values) when placed under the same physical circumstances (same  $H$ )

note: if the 2 particles are identical then their total  $H$  must not depend on our choice of labels  $\rightarrow H$  must be symmetric under exchange. Note: true for fermions too!

Example: consider 2 noninteracting particles, each described by the same nondegenerate Hamiltonian  $H_i$ , so that the total  $H = H_1 + H_2$

for example: 2 noninteracting particles in the same 1D square well.

For 2 distinguishable particles  $H$  may or may not be symmetric under exchange. Here we assume it is, for simplicity

If  $|\varepsilon_j\rangle, \varepsilon_j$  are the (nondeg.) eigenstates/values of each  $H_i$ , then

- for distinguishable particles, the eigenstates/values of  $H = H_1 + H_2$  include all possible combinations  $|\varepsilon_j\rangle|\varepsilon_k\rangle$ , w/ eigenvalues  $\varepsilon_j + \varepsilon_k$
- In particular, the 1<sup>st</sup> few eigenvalues/states of  $H$  are

$$E_1^D = 2\varepsilon_1 : \text{nondegenerate} ; \text{eigstate } |\varepsilon_1\rangle_1 |\varepsilon_1\rangle_2$$

$$E_2^D = \varepsilon_1 + \varepsilon_2 : 2\times \text{degenerate} ; \text{eigstates } |\varepsilon_1\rangle_1 |\varepsilon_2\rangle_2 \text{ or } |\varepsilon_2\rangle_1 |\varepsilon_1\rangle_2$$

if  $\epsilon_1 + \epsilon_3 < 2\epsilon_2$  :  $E_3^D = \epsilon_1 + \epsilon_3$  : 2x degenerate ; eigstates  $|\epsilon_1\rangle_1 |\epsilon_3\rangle_2$  or  $|\epsilon_3\rangle_1 |\epsilon_1\rangle_2$

if  $\epsilon_1 + \epsilon_3 > 2\epsilon_2$  :  $E_3^D = 2\epsilon_2$  : nondegenerate ; eigstate  $= |\epsilon_1\rangle_1 |\epsilon_2\rangle_2$

if  $\epsilon_1 + \epsilon_3 = 2\epsilon_2$  :  $E_3^D = \epsilon_1 + \epsilon_3 = 2\epsilon_2$  : 3x degenerate ; eigstates  $|\epsilon_1\epsilon_3\rangle, |\epsilon_3\epsilon_1\rangle, |\epsilon_2\epsilon_2\rangle$

for bosons : only symmetric combinations can appear

$E_1^B = 2\epsilon_1$  : nondegenerate ; eigstate  $|\epsilon_1\rangle_1 |\epsilon_1\rangle_2$

$E_2^B = \epsilon_1 + \epsilon_2$  : nondegenerate ; eigstate  $\frac{1}{\sqrt{2}} [|\epsilon_1\rangle_1 |\epsilon_2\rangle_2 + |\epsilon_2\rangle_1 |\epsilon_1\rangle_2]$

if  $\epsilon_1 + \epsilon_3 < 2\epsilon_2$  :  $E_3^B = \epsilon_1 + \epsilon_3$  : nondegenerate ; eigstate  $\frac{1}{\sqrt{2}} [|\epsilon_1\rangle_1 |\epsilon_3\rangle_2 + |\epsilon_3\rangle_1 |\epsilon_1\rangle_2]$

if  $\epsilon_1 + \epsilon_3 > 2\epsilon_2$  :  $E_3^B = 2\epsilon_2$  : nondegenerate ; eigstate  $= |\epsilon_1\rangle_1 |\epsilon_2\rangle_2$

if  $\epsilon_1 + \epsilon_3 = 2\epsilon_2$  :  $E_3^D = \epsilon_1 + \epsilon_3 = 2\epsilon_2$  : 2x degenerate ; eigstates  $\frac{1}{\sqrt{2}} [|\epsilon_1\epsilon_3\rangle + |\epsilon_3\epsilon_1\rangle], |\epsilon_2\epsilon_2\rangle$

for fermions : only antisymmetric combinations can appear

$E_1^F = \epsilon_1 + \epsilon_2$  : nondegenerate, eigstate  $\frac{1}{\sqrt{2}} [|\epsilon_1\rangle_1 |\epsilon_2\rangle_2 - |\epsilon_2\rangle_1 |\epsilon_1\rangle_2]$

if  $\epsilon_1 + \epsilon_3 < 2\epsilon_2$ ,  $\epsilon_1 + \epsilon_3 > 2\epsilon_2$  or  $\epsilon_1 + \epsilon_3 = 2\epsilon_2$  (regardless!)

$E_2^F = \epsilon_1 + \epsilon_3$ , nondegenerate eigstate  $\frac{1}{\sqrt{2}} [|\epsilon_1\rangle_1 |\epsilon_3\rangle_2 - |\epsilon_3\rangle_1 |\epsilon_1\rangle_2]$

ii) "Effective forces" due to symmetrization/antisymmetrization

Consider 2 particles moving in 1D one of which is in a position state  $|4\rangle$  and the other in a position state  $|4\rangle$  that is orthogonal to  $|4\rangle$

Consider 3 ways this can happen

a) Particle 1 in  $|4\rangle$ , particle 2 in  $|4\rangle$ :  $|4\rangle|4\rangle_2$

[this assumes the particles are distinguishable]

b) Symmetric state:  $\frac{1}{\sqrt{2}} [ |4\rangle|4\rangle + |4\rangle|4\rangle ]$

c) Antisym state:  $\frac{1}{\sqrt{2}} [ |4\rangle|4\rangle - |4\rangle|4\rangle ]$

Let us compare the average (squared) distance between the particles in each case:

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

Case a:  $\langle (x_1 - x_2)^2 \rangle_D = \langle \psi | x^2 | \psi \rangle - \langle \psi | \psi \rangle^2 + \langle \psi | \psi \rangle \langle \psi | x^2 | \psi \rangle - 2 \langle \psi | x | \psi \rangle \langle \psi | x | \psi \rangle$

$$= \langle x^2 \rangle_\psi + \langle x^2 \rangle_\psi - 2 \langle x \rangle_\psi \langle x \rangle_\psi$$

Case b:  $\langle (x_1 - x_2)^2 \rangle_s = \frac{1}{4} \left[ \begin{array}{cc} (\text{I}) & (\text{II}) \\ \langle \psi | \langle \psi | (x_1 - x_2)^2 | \psi \rangle | \psi \rangle + \langle \psi | \langle \psi | (x_1 - x_2)^2 | \psi \rangle | \psi \rangle & \\ & \\ & \text{III} \end{array} \right]$

$$+ \underbrace{\langle \psi | \langle \psi | (x_1 - x_2)^2 | \psi \rangle | \psi \rangle}_{(\text{III})} \pm \underbrace{\langle \psi | \langle \psi | (x_1 - x_2)^2 | \psi \rangle | \psi \rangle}_{(\text{IV})}$$

Terms I & II are equal to each other (note  $(x_1 - x_2)^2$  is symmetric under  $1 \leftrightarrow 2$ ) and also equal to the term from case a ( $= \langle (x_1 - x_2)^2 \rangle_D$ )

Terms III and IV are also equal to each other, and give

$$\begin{aligned} III = IV &= \langle \psi | x^2 | \psi \rangle \langle \psi | \psi \rangle + \langle \psi | \psi \rangle \langle \psi | x^2 | \psi \rangle - 2 \langle \psi | x | \psi \rangle \langle \psi | x | \psi \rangle \\ &= -2 |\langle \psi | x | \psi \rangle|^2 \end{aligned}$$

$$\boxed{\langle (x_1 - x_2)^2 \rangle_s = \langle (x_1 - x_2)^2 \rangle_D - 2 |\langle \psi | x | \psi \rangle|^2}$$

In words:

two particles in a symmetric (resp., antisymmetric) state are, on average, closer together (resp.: farther apart) than they would be in the corresponding product state

In a sense, the symmetrization postulate thus functions somewhat like a force (repulsive in the case of antisymmetric position states, and attractive in the case of symmetric ones). This is not really an accurate description of this effect, though, as there is no energy involved (the Hamiltonian remains the same in all cases).

Nevertheless, it has real physical consequences: the repulsive-like 'degeneracy pressure' between (fermionic) neutrons is what keeps a neutron star from collapsing under its own gravity. It (and not ordinary electrostatic repulsion) has also been shown to be the main reason preventing solid objects from passing through each other.

Note the extra term  $|\langle \psi | x | \varphi \rangle|^2$  vanishes if  $\psi(x), \varphi(x)$  have zero overlap in any region



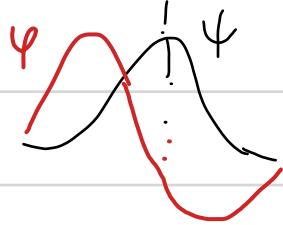
- in this case  $\langle \psi | x | \varphi \rangle = \int \psi^*(x) \varphi(x) x dx = 0$

In this situation then, there is no difference between the behaviour of bosons, fermions or distinguishable particles. We will generalize this observation below.

Comment: in contrast, an example where  $\langle \psi | \varphi \rangle = 0$  but  $\psi(x)$  and  $\varphi(x)$  are nonzero in the same region happens when  $\psi(x)$  is symmetric in  $x$  [ $\psi(x) = \psi(-x)$ ] but  $\varphi(x)$  is antisymmetric [ $\varphi(x) = -\varphi(-x)$ ]. In this case in general  $\langle \psi | x | \varphi \rangle \neq 0$ , and

bosons, fermions and distinguishable particles behave very differently.

ex:

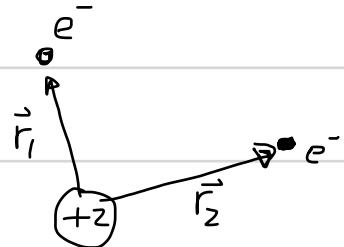


Application: Helium atom [see Gr. 5.11 for more, and Cohen Comp. BXIV for much more!]

The Helium atom has two electrons, which are of course fermions

Its Hamiltonian is:

$$H = \sum_{j=1}^2 \underbrace{\left[ -\frac{\hbar^2}{2m} \nabla_j^2 - k \cdot \frac{2e^2}{r_j} \right]}_{\text{2 Hydrogen-like terms with double nuclear charge}} + \underbrace{\frac{k e^2}{|\vec{r}_1 - \vec{r}_2|}}_{e^-e^- \text{ repulsion (correction)}}$$



Problem: impossible to solve analytically!

Later we will study some methods that allow pretty good approximate solutions

For now though: assume we can just ignore the  $e^-e^-$  repulsion term.

In this approximation, the eigenfunctions will just have the form of hydrogen-like wavefunctions  $\psi_{\text{He}}(\vec{r})$  for each electron

(these are rescaled versions of the Hydrogen wf's with half the Bohr radius and  $Z^2 = 4$  times the Bohr energy. See Hydrogenic ions discussion in QM1)

In this approximation, the ground state for He must then have both electrons in a  $1s$  state:

$$\Psi_{\text{ground}}^{\text{He}}(\vec{r}_1, \vec{r}_2) = \psi_{1s}(r_1) \psi_{1s}(r_2) \otimes \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$$

(since the spatial state is symmetric under  $1 \leftrightarrow 2$ , the electron spins must be in an antisymmetric state, ie, the singlet)

What about the 1<sup>st</sup> excited state though? Clearly, 1 electron should remain in its individual 1s state, while the other is excited to a 2s-type state

But: the 2 electron state must be antisymmetric overall. There are 2 ways to do this

$$\psi_{\text{OH}}^{\text{He}}(\vec{r}_1, \vec{r}_2) = \underbrace{\frac{1}{\sqrt{2}} [\psi_{1-0}(\vec{r}_1) \psi_{200}(\vec{r}_2) - \psi_{200}(\vec{r}_1) \psi_{100}(\vec{r}_2)]}_{\text{antisym}} \otimes \underbrace{[\text{triplet spin state}]}_{\text{sym}}$$

or

$$\psi_{\text{PH}}^{\text{He}}(\vec{r}_1, \vec{r}_2) = \underbrace{\frac{1}{\sqrt{2}} [\psi_{1-0}(\vec{r}_1) \psi_{200}(\vec{r}_2) + \psi_{200}(\vec{r}_1) \psi_{100}(\vec{r}_2)]}_{\text{sym}} \otimes \underbrace{[\text{singlet spin state}]}_{\text{antisym}}$$

The 1<sup>st</sup> type is known as an "ortho-helium" state, and the 2<sup>nd</sup> type is a "para-helium" state. By the argument we gave previously (which extends easily to 3D) in the symmetric "para-helium" spatial wavefunction, the electrons are closer together than in the antisymmetric "ortho-helium" ( $\langle |\vec{r}_1 - \vec{r}_2|^2 \rangle$  is smaller in para-helium).

In the absence of the  $e^-e^-$  repulsion, this wouldn't make any difference: both states would be stationary states with the same (degenerate) energy ( $E_1 + E_2$ )

However: repulsion does exist, and gives a contribution to the total energy that is i) positive ( $\frac{e^2}{|\vec{r}_1 - \vec{r}_2|} > 0$ ) and

ii) falls with the distance between  $e^-$ 's.

→ states where the electrons are further apart will have lower energy!

Now: in symmetric states, the avg distance  $\langle(\vec{r}_1 - \vec{r}_2)^2\rangle$  is smaller than the one in the corresponding antisymmetric state (as we have seen above). This means that the repulsion terms are stronger in parahelium than in orthohelium  $\rightarrow$  thus, parahelium states should (and actually do!) have higher energy than the corresponding orthohelium states.

In particular: the true 1<sup>st</sup> excited state is an orthohelium state similar to  $\psi_{^3\text{He}}(\vec{r}_1, \vec{r}_2)$  above!

$\rightarrow$  see Fig. 5.2 in Griffiths

Note: the actual eigenstates of para/ortho helium are not exactly the simple symmetric/antisym wf's above. However, the true wf's do have the same symmetry properties, so our constructions are good 1<sup>st</sup> approximations. We will see better ones later.

## General consequences of indistinguishability on physical predictions [CT D-2]

Suppose 2 particles (distinguishable, for now) are in orthogonal states  $|+\rangle, |-\rangle$ , and we wish to measure on both of them some single-particle observable  $B$ , with (for simplicity) nondegenerate possible values  $b_i$ .

Q: What is the probability of measuring a certain value  $b_i$  on one particle and  $b_j \neq b_i$  on the other? [without caring which is which]

[F. example:  $B$  can be  $S_z$ , ie, we can ask "what is the probability of measuring  $b_1 = +\frac{1}{2}$  on one particle and  $b_2 = -\frac{1}{2}$  on the other?"

$$A: P_B(b_i, b_j) = \underbrace{|\langle b_i b_j | + + \rangle|^2 + |\langle b_j b_i | + + \rangle|^2}_{\text{sum over 2 different ways this can happen}} = |\langle b_i | + \rangle|^2 |\langle b_j | + \rangle|^2 + |\langle b_j | + \rangle|^2 |\langle b_i | + \rangle|^2$$

Note: we would of course get the same result if the state were  $|+\rangle|-\rangle$  instead

What if the particles are bosons/fermions?

In this case, the symmetrization postulate says the joint state of the 2 particles must in fact be

$$|\chi_B\rangle_F = \frac{1}{\sqrt{2}} [ |+\rangle|-\rangle \pm |-\rangle|+\rangle]$$

Also, the amplitude should be calculated on a final state that is also properly (anti)symmetrized

$$\langle b_i b_j |^B_F = \frac{1}{\sqrt{2}} [\langle b_i b_j | \pm \langle b_j b_i |]$$

$$\rightarrow P_B(b_i, b_j) = \left| \langle b_i b_j | \chi_F \rangle \right|^2 = \left| \frac{1}{2} \left[ \langle b_i | \psi \rangle \langle b_j | \psi \rangle + \langle b_j | \psi \rangle \langle b_i | \psi \rangle \pm \langle b_i | \psi \rangle \langle b_j | \psi \rangle + \langle b_j | \psi \rangle \langle b_i | \psi \rangle \right] \right|^2$$

$$= \left| \langle b_i | \psi \rangle \langle b_j | \psi \rangle \pm \langle b_j | \psi \rangle \langle b_i | \psi \rangle \right|^2 \quad (*)$$

$P_B(b_i, b_j) = \underbrace{\left  \langle b_i   \psi \rangle \right ^2 \left  \langle b_j   \psi \rangle \right ^2}_{P_D(b_i, b_j)} + \underbrace{\left  \langle b_j   \psi \rangle \right ^2 \left  \langle b_i   \psi \rangle \right ^2}_{\text{exchange interference term}} \pm \underbrace{2 \operatorname{Re}(\langle b_j   \psi \rangle \langle \psi   b_i \rangle \langle b_i   \psi \rangle \langle \psi   b_j \rangle)}_{\text{exchange interference term}}$
---

Interpretation of (\*): for bosons/fermions, there are 2 indistinguishable 'paths' by which 2 particles initially in states  $|1\psi\rangle, |1\psi\rangle$  can be found in states  $|1b_i\rangle, |1b_j\rangle$

$$|\psi\rangle \rightarrow |b_i\rangle \quad \text{or} \quad |\psi\rangle \xrightarrow{} |b_i\rangle$$

$$|\psi\rangle \rightarrow |b_j\rangle \quad |\psi\rangle \xrightarrow{} |b_j\rangle$$

Because these two paths are indistinguishable, one must first sum the amplitude for each path and only then take the square modulus to calculate the probability  
 $\rightarrow$  analogous in this way to the double-slit experiment!

Example: consider two spin- $\frac{1}{2}$  particles in a state where one is in  $|+\rangle$  and the other is in  $|-\rangle$ . If we measure  $S_x$  for each particle, what is the probability of finding one with  $S_x = +\frac{\hbar}{2}$ , and the other with  $S_x = -\frac{\hbar}{2}$ ?

If the particles are distinguishable, in a state such as  $|+\rangle_1 |-\rangle_2$ , then

$$P_D(+\frac{\hbar}{2}, -\frac{\hbar}{2}) = \left| \langle +_x | + \rangle \right|^2 \left| \langle -_x | - \rangle \right|^2 + \left| \langle -_x | + \rangle \right|^2 \left| \langle +_x | - \rangle \right|^2 = 2 \cdot \left( \frac{1}{2} \cdot \frac{1}{2} \right) = \frac{1}{2}$$

If the particles are fermions (eg electrons) however, their state must be

$$|+-\rangle_A = \frac{1}{\sqrt{2}} [ |+-\rangle - |-+\rangle ] = \frac{1}{\sqrt{2}} [ |+_{x-x}\rangle - |-_{x+x}\rangle ] \quad (\text{same form in both bases!})$$

$$\begin{aligned} \text{and so : } P_F(+\frac{\hbar}{2}, -\frac{\hbar}{2}) &= P_D(+\frac{\hbar}{2}, -\frac{\hbar}{2}) - 2 \operatorname{Re} \left[ \underbrace{\langle +_x | +_x \rangle}_{-\frac{1}{\sqrt{2}}} \underbrace{\langle -_x | -_x \rangle}_{\frac{1}{\sqrt{2}}} - \underbrace{\frac{1}{\sqrt{2}} \cdot \frac{1}{\sqrt{2}}}_{-1} \right] \\ &= \frac{1}{2} + \frac{1}{2} = 1 ! \end{aligned}$$

This is easy to understand: the antisymmetric state is of course the singlet, for which there is no total angular momentum. In particular, every time we measure  $S_{x1} = +\frac{\hbar}{2}$ , we must also find  $S_{x2} = -\frac{\hbar}{2}$ , and vice-versa!

Here we can see this as an interference effect: although each state  $|+-\rangle$  and  $|-+\rangle$  have nonzero amplitudes for, say,  $|+_{x+x}\rangle$  and  $|-_{x-x}\rangle$ , these cancel each other due to the antisymmetric phase factor.

What about bosons? Of course, we know that spin- $\frac{1}{2}$  bosons don't really exist in Nature. Nevertheless, we can still consider an analogous question if we reinterpret  $|\pm\rangle$  as (eg)  $|S_z = \pm\frac{\hbar}{2}\rangle$ , and measure an observable  $S'$  for which  $\frac{|+\rangle + |-\rangle}{\sqrt{2}}$  are eigenstates with eigenvalue  $\pm\frac{\hbar}{2}$  (this observable is not  $S_x$  though)

Thus, for bosons the state is symmetric:  $\frac{1}{\sqrt{2}} [ |+-\rangle + |-+\rangle ] = \frac{1}{\sqrt{2}} [ |+_{x+x}\rangle - |-_{x-x}\rangle ]$   
(recall problem sheet 1!)  $\rightarrow$  we can see that here  $P(\frac{\hbar}{2}, -\frac{\hbar}{2}) = 0$

$$\text{Indeed : } P_B(\frac{\hbar}{2}, -\frac{\hbar}{2}) = \underbrace{P_D(\frac{\hbar}{2}, -\frac{\hbar}{2})}_{\frac{1}{\sqrt{2}}} + 2 \operatorname{Re} \left[ \underbrace{\langle +_x | +_x \rangle}_{-\frac{1}{\sqrt{2}}} \underbrace{\langle -_x | -_x \rangle}_{\frac{1}{\sqrt{2}}} - \underbrace{\frac{1}{\sqrt{2}} \cdot \frac{1}{\sqrt{2}}}_{-1} \right] = 0$$

- What about if  $b_i = b_j$ ? For distinguishable particles, the prob. of finding both in  $|b_i\rangle$  is

$$P_D(b_i, b_i) = |\langle b_i b_i | \psi \psi \rangle|^2 = |\langle b_i | \psi \rangle|^2 |\langle b_i | \psi \rangle|^2$$

For bosons : 
$$P_B(b_i, b_i) = \frac{1}{2} |\langle b_i b_i | (| \psi \psi \rangle + | \psi \psi \rangle) \rangle|^2 = \frac{1}{2} |2 \langle b_i | \psi \rangle \langle b_i | \psi \rangle|^2 = 2 P_D(b_i, b_i)$$

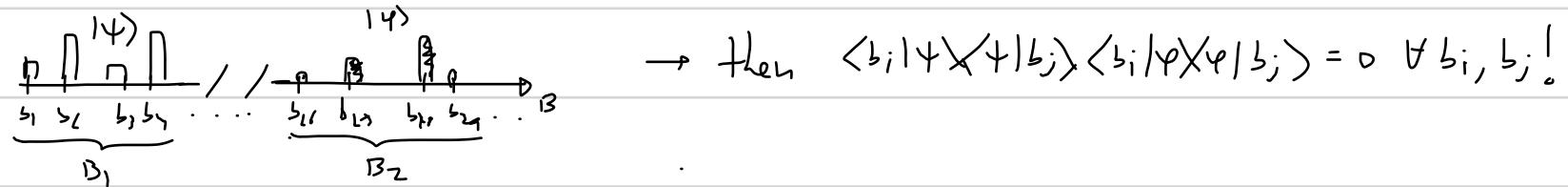
→ bosons are twice as likely to be found in the same state!

Of course, for fermions  $P_F(b_i, b_i) = \frac{1}{2} |\langle b_i b_i | (| \psi \psi \rangle - | \psi \psi \rangle) \rangle|^2 = 0$

- When is indistinguishability irrelevant?

In the example above, the fact that the particles are bosons/fermions becomes irrelevant if the exchange interference term always vanishes for any pair  $b_i, b_j$

This can only happen if there exist 2 disjoint sets of  $b_i$ 's  $B_1 = \{b_{i_1}, \dots, b_{i_m}\}$  and  $B_2 = \{b_{j_1}, \dots, b_{j_n}\}$  s.t.  $|\psi\rangle, |\psi\rangle$  only have amplitude ≠ 0 in  $B_1$  and  $B_2$ , respectively



- example: suppose  $|+\rangle, |-\rangle$  are initial states with completely disjoint wf's  $\psi(\vec{r})$  and  $\varphi(\vec{r})$

$$\bigcap_{|+\rangle} \quad \bigcap_{|-\rangle}$$

Then any measurements that are localized in space will behave as if the two particles were distinguishable. In other words, their positions is what distinguishes them!

- example: suppose  $|+\rangle, |-\rangle$  are spin+spatial states with orthogonal spin parts

$$\text{ex: } |+\rangle = |\psi_{esp}\rangle \otimes |+\rangle \quad ; \quad |-\rangle = |\varphi_{esp}\rangle \otimes |->$$

$$\rightarrow \text{full state for fermions: } \underbrace{\frac{1}{\sqrt{2}} \left[ |\psi_{esp}\rangle |\psi_{esp}\rangle_2 |+-\rangle_{12} - |\varphi_{esp}\rangle |\varphi_{esp}\rangle_2 |-+\rangle_{12} \right]}_{\text{P}} \quad \text{orthogonal}$$

Then even if the wavefunctions  $\psi_{esp}(\vec{r})$  and  $\varphi_{esp}(\vec{r})$  do have overlap, the particles will still behave, for spatial measurements, as if they were distinguishable — indeed, they are distinguishable precisely by their spin!

To see this, we need to extend our previous formalism to situations where  $B$  may have degeneracies. (This is the case here, since every spatial position  $\vec{r}$  corresponds to two eigenstates:  $|\vec{r}+\rangle$  and  $|\vec{r}-\rangle$ ).

In general, if for each value  $b_i$  we can have  $n_i$  eigenstates  $|b_i, k_i\rangle$ ,  $k_i=1\dots n_i$ , then to calculate  $P(b_i, b_j)$  we must sum over all possible combinations:

$$P(b_i, b_j) = \sum_{k_i=1}^{n_i} \sum_{k_j=1}^{n_j} \left| \langle b_i, k_i; b_j, k_j | \chi_B \rangle \right|^2$$

Expanding out each term in this sum, we find that the 'exchange interference term' becomes

$$\sum_{k_i} \sum_{k_j} 2 \operatorname{Re} \left( \langle b_{j,k_j} | \psi \rangle \langle \psi | b_{i,k_i} \rangle \langle b_{i,k_i} | \varphi \rangle \langle \varphi | b_{j,k_j} \rangle \right)$$

Returning to the example:  $B \equiv X$ ;  $b_i \equiv x$ ;  $|b_{i,1}\rangle \equiv |x,+\rangle$ ;  $|b_{i,2}\rangle \equiv |x,-\rangle$   
 $|\psi\rangle \equiv |\Psi_{esp}+\rangle$ ;  $|\varphi\rangle \equiv |\Psi_{esp}-\rangle$

So the probability (density) of finding one particle at  $x$  and the other at  $x'$  is

$$P(x, x') = |\Psi_{esp}(x)|^2 |\Psi_{esp}(x')|^2 + |\Psi_{esp}(x)|^2 |\Psi_{esp}(x')|^2 + \text{interference term}$$

where the interference term (for fermions) is

$$-2 \operatorname{Re} \left[ \begin{aligned} & \langle x' + | \Psi_{esp}+ \rangle \langle \Psi_{esp}+ | x + \rangle \langle x + | \cancel{\Psi_{esp}-} \rangle \langle \cancel{\Psi_{esp}-} | x' + \rangle \\ & + \langle x' + | \Psi_{esp}+ \rangle \langle \cancel{\Psi_{esp}+} | x - \rangle \langle \cancel{x -} | \Psi_{esp}- \rangle \langle \cancel{\Psi_{esp}-} | x' + \rangle \\ & + \langle x' - | \cancel{\Psi_{esp}+} \rangle \langle \Psi_{esp}+ | x + \rangle \langle \cancel{x +} | \cancel{\Psi_{esp}-} \rangle \langle \cancel{\Psi_{esp}-} | x' - \rangle \\ & + \langle x' - | \cancel{\Psi_{esp}+} \rangle \langle \cancel{\Psi_{esp}+} | x - \rangle \langle \cancel{x -} | \Psi_{esp}- \rangle \langle \cancel{\Psi_{esp}-} | x' - \rangle \end{aligned} \right] = 0$$

→ no exchange interference occurs!

Note: this may not remain true over time if the spin and spatial degrees of freedom of each particle interact, or if the 2 particles interact with each other.

General discussion: effect of symmetrization/antisymmetrization of N particles

'Recipe' for constructing general bosonic/fermionic states of N particles

- start by treating particles as if they are distinguishable

$$\text{ex } |\Psi_a\rangle_1 |\Psi_b\rangle_2 \cdots |\Psi_c\rangle_n = |\Psi_{a,b,\dots,c}^D\rangle$$

→ For bosons : Symmetrize the state, by summing over all permutations and normalizing

$$|\Psi_{a,b,\dots,c}^B\rangle = N_B \sum_{n! \text{ permutations}} (\text{all } n! \text{ permutations of } |\Psi_{a,b,\dots,c}\rangle)$$

Note that it does not matter what the ordering of states a...c was in the beginning, the final state is the same. All that matters is how many times each different state appears in the combination above

$$\text{ex: if } |\Psi_1^D\rangle = |\Psi_a\rangle |\Psi_b\rangle |\Psi_c\rangle, a,b,c \text{ different, or } |\Psi_2^D\rangle = |\Psi_c\rangle |\Psi_b\rangle |\Psi_a\rangle$$

$$\text{in both cases } |\Psi^B\rangle = \frac{1}{\sqrt{6}} [|\text{abc}\rangle + |\text{acb}\rangle + |\text{bac}\rangle + |\text{bca}\rangle + |\text{cab}\rangle + |\text{cba}\rangle]$$

$$\text{if } |\Psi_1^D\rangle = |\Psi_a\rangle |\Psi_a\rangle |\Psi_b\rangle, a,b \text{ different or } |\Psi_2^D\rangle = |\Psi_b\rangle |\Psi_a\rangle |\Psi_a\rangle$$

$$\text{in both cases } |\Psi^B\rangle = \frac{1}{\sqrt{3}} [|\text{baa}\rangle + |\text{aba}\rangle + |\text{aab}\rangle]$$

→ For fermions:

We must now Antisymmetrize the state, by summing over all permutations, adding a (-) sign according to the parity of the permutation (+1 if the permutation can be realized by an even numbers of swaps ('transpositions'), -1 if this number is odd)

$$|\Psi_{ab\ldots l}^B\rangle = N_B \sum_{n! \text{ permutations}}^{\text{Parity of the permutation}} (-1)^{\text{Parity of the permutation}} (\text{all } n! \text{ permutations of } |\Psi_{ab\ldots l}\rangle)$$

Again, it does not matter what the ordering of states  $a \dots l$  was in the beginning, the final state is the same (possibly up to a global (-) sign). All that matters is how many times each different state appears in the combination  $|\Psi_{a\ldots l}\rangle$

ex: if  $|\Psi_1^D\rangle = |\Psi_a\rangle|\Psi_b\rangle|\Psi_c\rangle$ ,  $a, b, c$  different, or  $|\Psi_2^D\rangle = |\Psi_c\rangle|\Psi_b\rangle|\Psi_a\rangle$

$$\text{in both cases } |\Psi^F\rangle = \frac{\pm 1}{\sqrt{6}} \left[ |\text{abc}\rangle - |\text{acb}\rangle + |\text{bca}\rangle - |\text{bac}\rangle + |\text{cab}\rangle - |\text{cba}\rangle \right]$$

if  $|\Psi_1^D\rangle = |\Psi_a\rangle|\Psi_a\rangle|\Psi_b\rangle$ ,  $a, b$  different or  $|\Psi_2^D\rangle = |\Psi_b\rangle|\Psi_a\rangle|\Psi_a\rangle$

$$\text{in both cases } |\Psi^F\rangle = \frac{\pm 1}{\sqrt{6}} \left[ |\text{aba}\rangle - |\text{aab}\rangle + |\text{baa}\rangle - |\text{baa}\rangle + |\text{aab}\rangle - |\text{aba}\rangle \right] = 0$$

There is a special trick to simplify the calculation of a fermionic state, known as the Slater determinant: given  $n$  individual states  $|\Psi_a\rangle, |\Psi_b\rangle, \dots |\Psi_n\rangle$  for  $n$  individual fermions, the properly antisymmetrized state can be written as:

$$|AS\rangle = \frac{1}{\sqrt{n!}} \begin{vmatrix} |\Psi_a\rangle_1 & |\Psi_b\rangle_1 & \dots & |\Psi_n\rangle_1 \\ |\Psi_a\rangle_2 & |\Psi_b\rangle_2 & \dots & |\Psi_n\rangle_2 \\ \vdots & \vdots & \ddots & \vdots \\ |\Psi_a\rangle_n & |\Psi_b\rangle_n & \dots & |\Psi_n\rangle_n \end{vmatrix} \quad (\text{sub-indexes inside the kets refer to which state; sub-indexes outside the kets refer to which particle})$$

Where we take tensor products between states when calculating the determinant. This works because determinants have exactly the same antisymmetry properties we require ( $\det \text{changes sign if we exchange 2 rows}$ )

Example : ground state of Lithium ( $Z=3$ )

Let us first ignore the electron-electron interaction, as we did above for Helium. Then we can approximate the eigenstates of the 3-electron system as [properly antisymmetrized] products of individual states for each electron

Due to spin, we can have 2 electrons with  $n=1$  ( $1s$  state), but the  $3^{\text{rd}}$  must have  $n=2$  (with spin either + or - ... let's choose +)

We must therefore antisymmetrize the state  $|1+\rangle_1 |1-\rangle_2 |2+\rangle_3$

$$|\text{Ligd state}\rangle = \frac{1}{\sqrt{3!}} \begin{vmatrix} |1+\rangle & |1-\rangle & |2+\rangle \\ |1+\rangle & |1-\rangle & |2+\rangle \\ |1+\rangle & |1-\rangle & |2+\rangle \end{vmatrix} = \frac{1}{\sqrt{6}} \begin{bmatrix} |112\rangle |+-+ \rangle - |121\rangle |++- \rangle + |121\rangle |-+ \rangle \\ - |112\rangle |-+ \rangle + |211\rangle |+- \rangle - |211\rangle |+- \rangle \end{bmatrix}$$

Note :

The description we gave above for the ground state is still incomplete - because we did not specify which  $n=2$  state should be occupied

In hydrogen, of course,  $2s$  and  $2p$  states [ $l=0$  or  $l=1$ ] have the same energy.

When there are more electrons, however, this is no longer true: for a given  $n$ , the states with lower  $l$  have lower energy. In other words: the " $|2s\rangle$ " state above is actually the  $|2s\rangle$  state ( $l=m=0$ )

This effect is actually due to the electron-electron repulsion (which we have been ignoring so far, remember?)

Later on in this course we will develop tools that will allow us to understand this effect better (both qualitatively and quantitatively)

## Occupation number notation

Since it doesn't matter which indistinguishable particle is in which state, only how many are in each state, a compact and powerful way to describe the state of a system of identical bosons or fermions is simply to count how many are in each (of a set of orthogonal) individual state

ex:  $|n_a, n_b, n_c\rangle$  represents a state of  $N = n_a + n_b + n_c$  bosons in which  $n_a$  of them are in state  $|a\rangle$ ,  $n_b$  of them in state  $|b\rangle$  &  $n_c$  in state  $|c\rangle$ .

this is shorthand for the state cte.  $\sum_{\text{all } n! \text{ permutations}}^{} |a_{\underbrace{\dots}_{n_a}, b_{\underbrace{\dots}_{n_b}, c_{\underbrace{\dots}_{n_c}}}\rangle$

The same works for fermions → however, in this case each  $n_a, b, c$  can only be equal to 0 or 1!

Ex: consider a system of  $N$  non-interacting particles, each subject to the same Hamiltonian  $H_j$ , so that

$$H = \sum H_j$$

Suppose for simplicity that  $H_j$  is non-degenerate, with ground state  $|0\rangle$  and 1<sup>st</sup> excited state  $|1\rangle$ . Then the gd state of an  $N$ -boson system is

$$|_{\text{ground}}\rangle_B = |0\rangle_1 \dots |0\rangle_N = |0, 0 \dots, 0\rangle$$

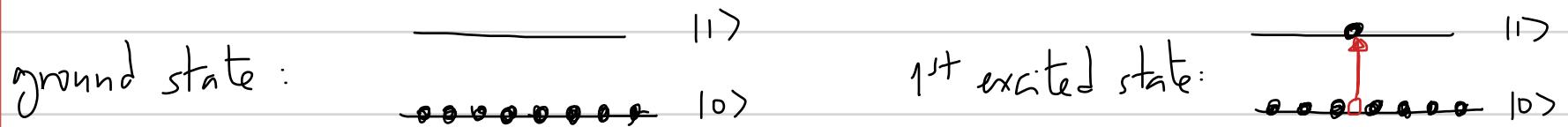
In occupation-number notation, this is  $|_{\text{ground}}\rangle_B = |n_0=N, n_j=0, \forall j>0\rangle$

The 1<sup>st</sup> excited state will have one excited boson. Because of symmetrization, we cannot tell which of the bosons is excited though. Thus this state is:

$$\text{In ordinary notation: } |\text{1 excited}\rangle_B = \frac{1}{\sqrt{N}} [ |1, 0, \dots, 0\rangle + |0, 1, 0, \dots, 0\rangle + \dots + \dots |0, 0, \dots, 0, 1\rangle ]$$

$$\text{In occupation number notation: } |\text{1 excited}\rangle_B = |n_0=N-1, n_1=1, n_j=0; \forall j > 1\rangle$$

In visual terms:



For fermions, however, we can only have  $n_j=0$  or  $1$

Thus, the ground state is the one where the  $N$  lowest levels have exactly 1 fermion:

$$\text{In occupation number notation } |\text{ground}\rangle_F = |n_0=1, n_1=1, \dots, n_{N-1}=1, n_j=0; j \geq N\rangle$$

In ordinary notation, we would have to construct the Slater determinant

$$\frac{1}{\sqrt{N!}} \begin{vmatrix} |0\rangle_1 |1\rangle_1 \dots |N-1\rangle_1 \\ |0\rangle_2 |1\rangle_2 \dots |N-1\rangle_2 \\ \vdots \\ |0\rangle_N |1\rangle_N \dots |N-1\rangle_N \end{vmatrix}$$

The 1<sup>st</sup> excited state is then the one where one fermion is in the next lowest possible level, and all the others are as low as possible

$$|1 \text{ excited}\rangle_F = |n_1=1, n_2=1 \dots n_{N-1}=1, n_N=0, n_{N+1}=1\rangle$$

In visual terms:

