

## 7 Identical Particles

### 7.1 Permutation symmetry

Identical particles  $\hat{=}$  indistinguishable particles



If particles 1 and particles 2 are identical, we don't know if the outcome of a reaction or scattering event is the situation on the left or the situation on the right: Particles 1 and 2 are indistinguishable and we cannot tell them apart.

If we call one particle 1 and the other particle 2, then these are just names — we don't really know which is which since we cannot distinguish them.

Say, we are considering a particle in state  $|g'\rangle$  and another particle in state  $|g''\rangle$ . If we are dealing with identical particles, the states

$|k'\rangle, |k''\rangle_2$  and  $|k''\rangle, |k'\rangle_2$  are not acceptable

states. We need to construct states that are consistent with the identical particle nature:

$$\left( \frac{1}{\sqrt{2}} (|k'\rangle, |k''\rangle_2 \pm |k''\rangle, |k'\rangle_2) \right)$$

normalization

identical bosons

identical fermions

What is the normalization factor about?

Let's assume:  $\langle k' | k' \rangle = 1$

$$\langle k'' | k'' \rangle = 1$$

since we are working w/ plane wave states, we have  $\langle k', k'' \rangle = \delta(k' - k'')$

Define  $|\psi\rangle = \frac{1}{\sqrt{2}} (|k'\rangle, |k''\rangle_2 \pm |k''\rangle, |k'\rangle_2)$  and work out

$$\langle \psi | \psi \rangle = \frac{1}{2} \left[ (\langle k' | k'' \rangle \pm \langle k'' | k' \rangle) (|k'\rangle, |k''\rangle_2 \pm |k''\rangle, |k'\rangle_2) \right]$$

$$= \frac{1}{2} \left[ \langle k' | k'' \rangle, \langle k'' | k' \rangle_2 + \langle k'' | k'' \rangle, \langle k' | k' \rangle_2 \right]$$

$$\pm \langle k'' | k' \rangle, \langle k' | k'' \rangle_2 \pm \langle k' | k'' \rangle, \langle k'' | k' \rangle_2 \right]$$

$$= \frac{1}{2} [ 1 \cdot 1 + 1 \cdot 1 \pm 0 \cdot 0 \pm 0 \cdot 0 ]$$

$$= 1$$

$\rightarrow$  the factor of  $\frac{1}{\sqrt{2}}$  ensures normalization

What is the  $\pm$  about?

Let's look at what happens when we exchange particles 1 and 2. This is accomplished by the operator  $\hat{P}_{12}$ :

$$\begin{aligned}\hat{P}_{12} |14\rangle &= \hat{P}_{12} \left[ \frac{1}{\sqrt{2}} (|1s'\rangle, |1s''\rangle_2 \pm |1s''\rangle, |1s'\rangle_2) \right] \\ &= \frac{1}{\sqrt{2}} \left[ |1s''\rangle, |1s'\rangle_2 \pm |1s'\rangle, |1s''\rangle_2 \right] \\ &= \pm \frac{1}{\sqrt{2}} (|1s'\rangle, |1s''\rangle_2 \pm |1s''\rangle, |1s'\rangle_2) \\ &= \pm |14\rangle\end{aligned}$$

$$\Rightarrow \frac{1}{\sqrt{2}} (|1s'\rangle, |1s''\rangle_2 + |1s''\rangle, |1s'\rangle_2)$$

is symmetric under  
the exchange of  
particles 1 and 2

$\hat{S}_{12} = \frac{1}{\sqrt{2}} (1 + \hat{P}_{12})$  is symmetrization operator

$$\hat{S}_{12} |1s'\rangle, |1s''\rangle_2 = \frac{1}{\sqrt{2}} (|1s'\rangle, |1s''\rangle_2 + |1s''\rangle, |1s'\rangle_2)$$

and  $\frac{1}{\sqrt{2}} (|1s'\rangle, |1s''\rangle_2 - |1s''\rangle, |1s'\rangle_2)$  is anti-symmetric under  
the exchange of particles  
1 and 2

$\hat{A}_{12} = \frac{1}{\sqrt{2}} (1 - \hat{P}_{12})$  is anti-symmetrization operator

$$\hat{A}_{12} |1s'\rangle, |1s''\rangle_2 = \frac{1}{\sqrt{2}} (|1s'\rangle, |1s''\rangle_2 - |1s''\rangle, |1s'\rangle_2)$$

From now on:  $|k'\rangle, |k''\rangle_2 \rightarrow |k'\rangle |k''\rangle$

i.e., we imply that the order is left for particle 1, left for particle 3, left for particle 3, ...

Importantly: the exchange symmetry (+ for identical bosons & - for identical fermions) has measurable consequences!

Why is matter stable? I.e., why can we construct a table that consists of a rather low density material and is stable?

- fermionic nature of matter
- Let's look at  $\psi(z_1, z_2)$  as an example.

$z_1$  = coordinate of particle 1.

$z_2$  = coordinate of particle 2.

Let's say that  $\psi(z_1, z_2)$  is anti-symmetric under the exchange of particles 1 and 2.

$$\Rightarrow \psi(z_1, z_2) = -\psi(z_2, z_1)$$

$$\text{Now: } z_1 = a, z_2 = a \text{ and } \psi(a, a) = A$$

$$\Rightarrow A = -A \Rightarrow A = 0$$

The probability to find particles 1 and particles 2 at the same location is zero.

→ The anti-symmetric wave fct. nature associated with identical fermions (here, electrons) makes the table stable → somehow, there needs to be an excluded volume → finite density.

## 7.2 Symmetrization postulate

$N$  identical particles in 3D (2D is a bit more subtle : there exists anyonic in 2D that interpolates smoothly between bosonic statistics and fermionic statistics)

→ you might have heard about an anyonic quantum computer and terms like braider)

Option 1: bosons

Option 2: fermions

(in 3D, no other options)

} What do we mean by options? The phenomena observed are such that they can be described by bosonic statistics or by fermionic statistics

Integer spin particles  $\hat{=}$  bosons

state must be totally symmetric under the exchange of any pair of identical particles:

$$\hat{P}_{ij} |"N\text{-particle state"}\rangle = + |"N\text{-particle state"}\rangle$$

Some ket that describes the  $N$ -particle system

$ij$  refer to any pair of particles

Bose-Einstein statistics

Half-integer spin particles  $\hat{=}$  fermions

state must be totally anti-symmetric under the exchange of any pair of identical particles:

$$\hat{P}_{ij} |"N\text{-particle state"}\rangle = - |"N\text{-particle state"}\rangle$$

Fermi-Dirac statistics

Electrons = fermions : electrons must obey the Pauli

exclusion principle : no two

electrons can occupy the same

state.

Note: the table ~~any~~ example discussed earlier used a simplified argument that only considers the spatial degrees of freedom. We must also consider spin!

Distinguishable particles: Maxwell - Boltzmann statistics

→ sometimes, we refer to distinguishable particles as "classical" particles  
 → the quantum statistical nature is no longer visible / measurable and the Bose-Einstein statistics and Fermi-Dirac statistics approach the Maxwell-Boltzmann statistics

Let's return to our two-particle example ( $|k'\rangle$  and  $|k''\rangle$ ):

① distinguishable particles:  $|k'\rangle |k''\rangle$

$$|k''\rangle |k'\rangle$$

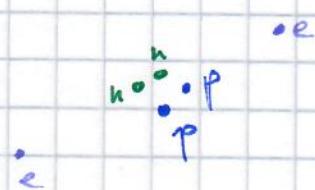
② identical bosons:  $\frac{1}{2}(|k'\rangle |k''\rangle + |k''\rangle |k'\rangle)$

③ identical fermions:  $\frac{1}{2}(|k'\rangle |k''\rangle - |k''\rangle |k'\rangle)$

Examples: fermions: electron  
 bosons: photon } elementary

But also composite particles:

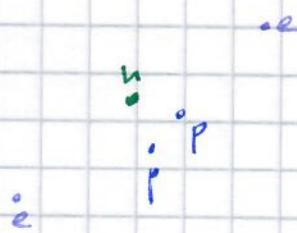
e.g.:  ${}^4\text{He}$



6 spin- $\frac{1}{2}$  particles

→ combine to integer spin (angular momentum addition)

${}^3\text{He}$



5 spin- $\frac{1}{2}$  particles

→ combine to half-integer spin

The low-temperature behavior of liquid helium-4 and liquid helium-3 is vastly different:

${}^4\text{He}$ : superfluid below 2.17 K

${}^3\text{He}$ : transition temperature is much lower  
 (millikelvin regime)

But what about the proton and neutron?

They are not elementary particles:

proton / neutron consists of three quarks



Quark  $\hat{=}$  elementary spin- $\frac{1}{2}$  particle

$\rightarrow$  3 spin- $\frac{1}{2}$  particles combine to half-integers spin

$\Rightarrow$  proton / neutron  $\hat{=}$  composite fermions

$\pi$ -meson  $\hat{=}$  composite boson (mesons consist of two quarks)

Question: If I give you a single particle, can you tell whether it is a fermion or a boson?

Answer: Unless you can measure spin (or the projection quantum number), we cannot tell  $\rightarrow$  the exchange statistics becomes "visible" when we add a second particle.

### 7.3 Two-electron system

Electron 1:  $\vec{x}_1, s_1, m_{s1}$

Electron 2:  $\vec{x}_2, s_2, m_{s2}$

$$\left. \begin{array}{l} s_1 = s_2 = \frac{1}{2} \\ \text{(will be dropped} \\ \text{in what follows)} \end{array} \right\}$$

Wave function:  $\Psi(\vec{x}_1, m_{s1}, \vec{x}_2, m_{s2})$

$$\hat{P}_{12} \Psi(\vec{x}_1, m_{s1}, \vec{x}_2, m_{s2}) = -\Psi(\vec{x}_2, m_{s2}, \vec{x}_1, m_{s1})$$



$\hat{P}_{12}$  exchanges the  
spatial and the spin  
degrees of freedom

We can write  $\hat{P}_{12} = \hat{P}_{12}^{(\text{space})} \hat{P}_{12}^{(\text{spin})}$

$$\hat{S}_{\text{tot}} = \hat{s}_1 + \hat{s}_2$$

If  $[\hat{S}_{\text{tot}}^2, \hat{H}] = 0$ , then we can find simultaneous eigenfunctions of  $\hat{H}$  and  $\hat{S}_{\text{tot}}^2$ .

$\hat{H}$ : system Hamiltonian (for now, this is quite general—any two-electron Hamiltonian; later, this will be the Hamiltonian of the helium atom).

What are eigenkets of  $\hat{S}_{\text{tot}}^2$ ?

$$|m_{s_1} = \frac{1}{2}, m_{s_2} = \frac{1}{2}\rangle$$

$$|-\frac{1}{2}, -\frac{1}{2}\rangle$$

$$\frac{1}{\sqrt{2}}(|+\frac{1}{2}, -\frac{1}{2}\rangle + |-\frac{1}{2}, +\frac{1}{2}\rangle)$$

$$\frac{1}{\sqrt{2}}(|+\frac{1}{2}, -\frac{1}{2}\rangle - |-\frac{1}{2}, +\frac{1}{2}\rangle)$$

}

triplet states  
( $S_{\text{tot}} = 1; M_{\text{tot}} = 0, \pm 1$ )

}

singlet state  
( $S_{\text{tot}} = 0; M_{\text{tot}} = 0$ )

Since  $\hat{\vec{S}}_1 \cdot \hat{\vec{S}}_2 | \text{singlet} \rangle = -\frac{3\hbar^2}{4} | \text{singlet} \rangle$

and  $\hat{\vec{S}}_1 \cdot \hat{\vec{S}}_2 | \text{triplet} \rangle = \frac{\hbar^2}{4} | \text{triplet} \rangle$ ,

we can write

$$\hat{P}_{12}^{(\text{spin})} = \frac{1}{2} \left( 1 + \frac{4}{\hbar^2} \hat{\vec{S}}_1 \cdot \hat{\vec{S}}_2 \right).$$

Let's write  $\alpha(\vec{x}_1, m_{s_1}, \vec{x}_2, m_{s_2}) = \underbrace{\phi(\vec{x}_1, \vec{x}_2)}_{\text{spatial part}} \underbrace{X(m_{s_1}, m_{s_2})}_{\text{spin part}}$

If  $|X\rangle = |\text{triplet}\rangle$ , then  $\hat{P}_{12}^{(\text{spatial})} \phi(\vec{x}_1, \vec{x}_2) = -\phi(\vec{x}_2, \vec{x}_1)$ .

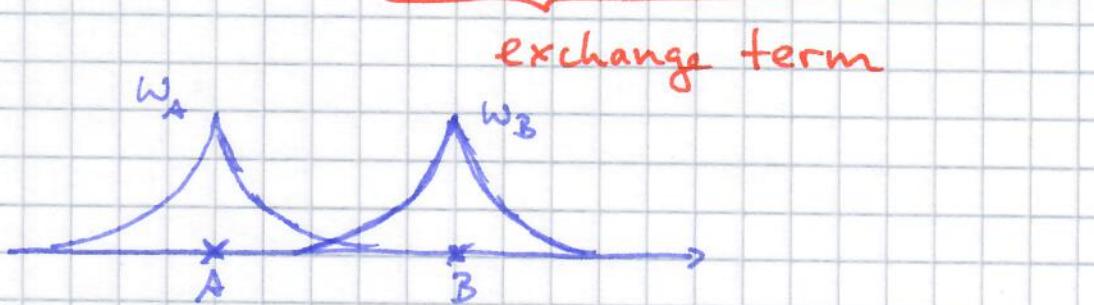
If  $|X\rangle = |\text{singlet}\rangle$ , then  $\hat{P}_{12}^{(\text{spatial})} \phi(\vec{x}_1, \vec{x}_2) = +\phi(\vec{x}_2, \vec{x}_1)$ .

As an example, let's look at a specific form of  $\phi(\vec{x}_1, \vec{x}_2)$ :

$$\phi(\vec{x}_1, \vec{x}_2) = \frac{1}{\sqrt{2}} \left[ w_A(\vec{x}_1) w_B(\vec{x}_2) \pm w_A(\vec{x}_2) w_B(\vec{x}_1) \right]$$

Let's calculate  $|\phi(\vec{x}_1, \vec{x}_2)|^2$ :

$$|\phi(\vec{x}_1, \vec{x}_2)|^2 = \frac{1}{2} \left[ |w_A(\vec{x}_1)|^2 |w_B(\vec{x}_2)|^2 + |w_A(\vec{x}_2)|^2 |w_B(\vec{x}_1)|^2 \right. \\ \left. \pm 2 \operatorname{Re} \left\{ w_A(\vec{x}_1) w_B(\vec{x}_2) w_A^*(\vec{x}_2) w_B^*(\vec{x}_1) \right\} \right]$$



A: point around which  $w_A$  is centered

B: point around which  $w_B$  is centered

If A and B are very far separated, the overlap between  $w_A$  and  $w_B$  decreases  $\Rightarrow$

The exchange term goes to zero

An electron on Earth and an electron on the Moon are uncorrelated, even though they are

identical).

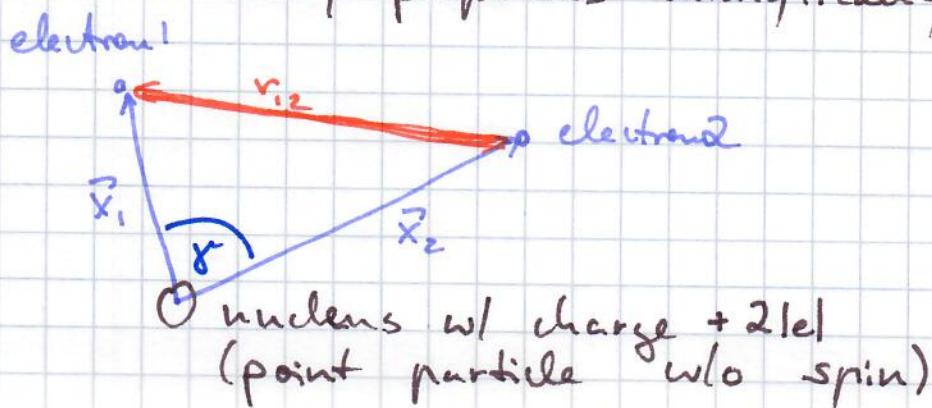
Eventually, for sufficiently large separation between A and B, electron 1 will be localized at A or B and electron 2 will be localized at the other spot (i.e., B or A).

#### 7.4 The helium atom

This section can be viewed as an application of the more general considerations discussed in Sec. 7.3.

Also: This section can be viewed as an application or review of time-independent perturbation theory.

In addition: Helium is the simplest of the "non-trivial" atoms ( $\rightarrow$  I'm referring to the H-atom as trivial since we can treat many properties analytically).



$$\hat{H} = \frac{\hat{p}_1^2}{2m} + \frac{\hat{p}_2^2}{2m} - \frac{2e^2}{r_1} - \frac{2e^2}{r_2} + \frac{e^2}{r_{12}}$$

Coulomb attraction  
between electron  
and nucleus

Coulomb attraction  
between electron 2  
and nucleus

Note:  
the Hamiltonian  
does not de-  
pend on spin  
→ only em  
interaction  
is included

$$r_1 = |\vec{x}_1|$$

$$r_2 = |\vec{x}_2|$$

$\hat{p}_1$ : momentum operator of electron 1

$\hat{p}_2$ : momentum operator of electron 2

m: electron mass

$$r_{12} = |\vec{x}_1 - \vec{x}_2|$$

Since  $[\hat{H}, \hat{S}_{\text{tot}}^2] = 0$ , we can write the wave functions (energy eigenkets) as a product of spatial part and spin part.

Let us assume for a moment that the electron-electron interaction can be neglected

(it turns out that it contributes of order 25%)

to the energy).

$$\text{Then: } \hat{H}_0 = \frac{\hat{p}_1^2}{2m} - \frac{2e^2}{r_1} + \frac{\hat{p}_2^2}{2m} - \frac{2e^2}{r_2}$$

hydrogenic  
 $z=2$  Hamiltonian  
for first electron
hydrogenic  $z=2$   
Hamiltonian for  
second electron

$\hat{H}_{e1}$                        $\hat{H}_{e2}$

The energy eigen sets can be obtained by separation of variables:

$$\Psi_{n_1' l_1' m_1'}(\vec{x}_1) \Psi_{n_2 l_2 m_2}(\vec{x}_2)$$

here:  $\Psi_{n l m} \stackrel{\cong}{=} \text{hydrogenic } z=2$   
wave fct.

Apply  $\hat{S}_{12}$  or  $\hat{A}_{12}$ :

for spin singlet

↑  
for spin triplet

$$\phi(\vec{x}_1, \vec{x}_2) = \frac{1}{\sqrt{2}} \left[ \Psi_{n_1' l_1' m_1'}(\vec{x}_1) \Psi_{n_2 l_2 m_2}(\vec{x}_2) \right. \\ \left. + \Psi_{n_1' l_1' m_1'}(\vec{x}_2) \Psi_{n_2 l_2 m_2}(\vec{x}_1) \right]$$

To make life a bit simpler, let us assume that one of the electrons is sitting in the

$n'=1$ ,  $\ell=0$ , and  $m_\ell=0$  orbital:

$$\rightarrow \phi(\vec{x}_1, \vec{x}_2) = \frac{1}{\sqrt{2}} \left[ \psi_{100}(\vec{x}_1) \psi_{100}(\vec{x}_2) \pm \psi_{100}(\vec{x}_2) \psi_{100}(\vec{x}_1) \right]$$

For ground state:  
("1s<sup>2</sup> configuration")

$$\phi_{\text{gr}}^{(0)}(\vec{x}_1, \vec{x}_2) = \frac{z^3}{\pi a_0^3} e^{-2r_1/a_0} e^{-2r_2/a_0}$$

Spin part: anti-symmetric  
(spin singlet)

$$\overline{E}_{\text{gr.}}^{(0)} = 2 \cdot z^2 (-13.6 \text{ eV}) = -108.8 \text{ eV}$$

$\uparrow$   
 $z=2$

The exact value is  
-78.8 eV.

So far, the electron-electron interaction has been neglected completely. We can account for it in an approximate manner by performing a first-order time-independent perturbation theory treatment.

Need to evaluate  $\int |\phi_{\text{gr}}^{(0)}(\vec{x}_1, \vec{x}_2)|^2 \frac{e^2}{r_{12}} d^3 \vec{x}_1 d^3 \vec{x}_2$

After some algebra and integration:

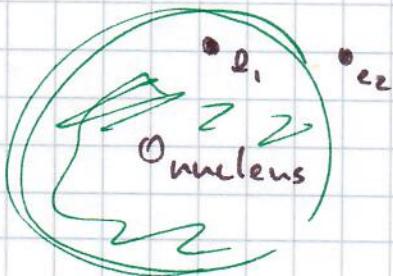
$$E_{\text{gr}}^{(0)} + \Delta E_{\text{gr}}^{(1)} = -74.8 \text{ eV}$$

recall the exact value is  
-78.8 eV.

Alternatively, we can pursue a variational approach.

What is the idea?

The idea is that the electrons may not see the charge of  $Z=2$  when the electron-electron interaction is turned on.



Variational wave function:

$$\langle \vec{x}_1, \vec{x}_2 | \bar{\psi} \rangle$$

$$= \frac{Z_{\text{eff}}^3}{\pi a_0^3} e^{-Z_{\text{eff}}(r_1+r_2)/a_0}$$

$Z_{\text{eff}} \hat{=} \text{variational parameter}$

the charge seen by electron 2 may be smaller than  $Z_{\text{el}}$  since the first electron might be screening the nuclear charge.

In particular, if electron 2 is very far away from nucleus plus electron 1, then it looks as though the "nucleus" (better the core) has a charge of  $1e$ .

$$E_{\text{var}}(z_{\text{eff}}) = \langle \bar{0} | \hat{H} | \bar{0} \rangle$$

↗  
full Hamiltonian  
(including electron-electron interaction)

$$= \dots$$

$$\text{Set } \frac{\partial E_{\text{var}}(z_{\text{eff}})}{z_{\text{eff}}} = 0 \Rightarrow z_{\text{eff}}^* = 1.6875$$

$$E_{\text{var}}(z_{\text{eff}}^*) = -77.5 \text{ eV}$$

recall: the exact value is  
-78.8 eV.

Let us now consider excited states. For this, we will return to

$$\phi(\vec{x}_1, \vec{x}_2) = \frac{1}{\sqrt{2}} \left[ \psi_{100}(\vec{x}_1) \psi_{nlm_2}(\vec{x}_2) \pm \psi_{100}(\vec{x}_2) \psi_{nlm_2}(\vec{x}_1) \right]$$

For an excited state:  $(nlm_2) \neq (1, 0, 0)$ .

Let's use TIPST:

$$E_{\text{exc}}^{(0)} = E_{100} + E_{nlm_2}$$

$$= -2^2 13.6 \text{ eV} + 2^2 \frac{-13.6 \text{ eV}}{n^2}$$

What about 1<sup>st</sup> order correction?

$$\Delta E_{\text{exc}}^{(1)} = \frac{1}{2} \int |\psi_{100}(\vec{x}_1)|^2 |\psi_{\text{helium}}(\vec{x}_2)|^2 \frac{e^2}{r_{12}} d^3 \vec{x}_1 d^3 \vec{x}_2$$

$$+ \frac{1}{2} \int |\psi_{100}(\vec{x}_2)|^2 |\psi_{\text{helium}}(\vec{x}_1)|^2 \frac{e^2}{r_{12}} d^3 \vec{x}_1 d^3 \vec{x}_2$$

$$\pm \frac{1}{2} \int \psi_{100}^*(\vec{x}_1) \psi_{\text{helium}}^*(\vec{x}_2) \psi_{100}(\vec{x}_2) \psi_{\text{helium}}(\vec{x}_1) \frac{e^2}{r_{12}} d^3 \vec{x}_1 d^3 \vec{x}_2$$

$$\pm \frac{1}{2} \int \psi_{100}^*(\vec{x}_2) \psi_{\text{helium}}^*(\vec{x}_1) \psi_{100}(\vec{x}_1) \psi_{\text{helium}}(\vec{x}_2) \frac{e^2}{r_{12}} d^3 \vec{x}_1 d^3 \vec{x}_2$$

Now: the coordinates  $\vec{x}_1$  and  $\vec{x}_2$  are being integrated over, i.e., they are dummy indices and we can rename

$\vec{x}_1 \rightarrow \vec{x}_2$  and  $\vec{x}_2 \rightarrow \vec{x}_1$  in the second blue integral and

in the second brown integral.

$$= \boxed{\int |\psi_{100}(\vec{x}_1)|^2 |\psi_{\text{helium}}(\vec{x}_2)|^2 \frac{e^2}{r_{12}} d^3 \vec{x}_1 d^3 \vec{x}_2} \quad \boxed{J}$$

$$\pm \boxed{\int \psi_{100}^*(\vec{x}_1) \psi_{\text{helium}}^*(\vec{x}_2) \psi_{100}(\vec{x}_2) \psi_{\text{helium}}(\vec{x}_1) \frac{e^2}{r_{12}} d^3 \vec{x}_1 d^3 \vec{x}_2}$$

$$\Rightarrow \Delta E_{\text{exc}}^{(1)} = J \pm \frac{1}{2}$$

$$\delta E_{\text{exc}}^{(1)} = E_{\text{exc}}^{(0)} + J \pm \frac{1}{2}$$

for spin singlet

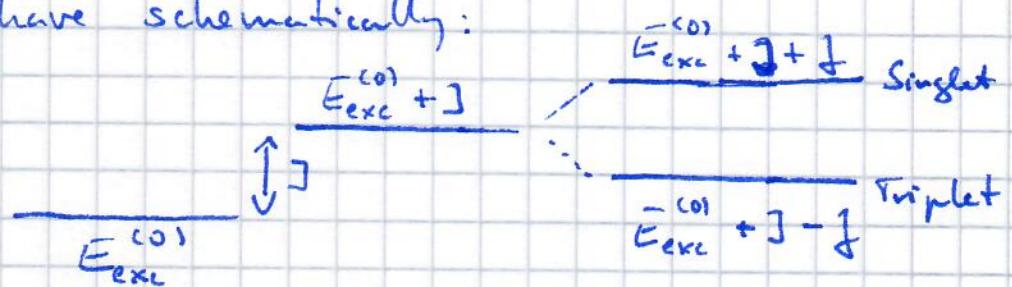
$\downarrow$

for spin triplet

It can be shown that  $\frac{1}{2}$  is positive.

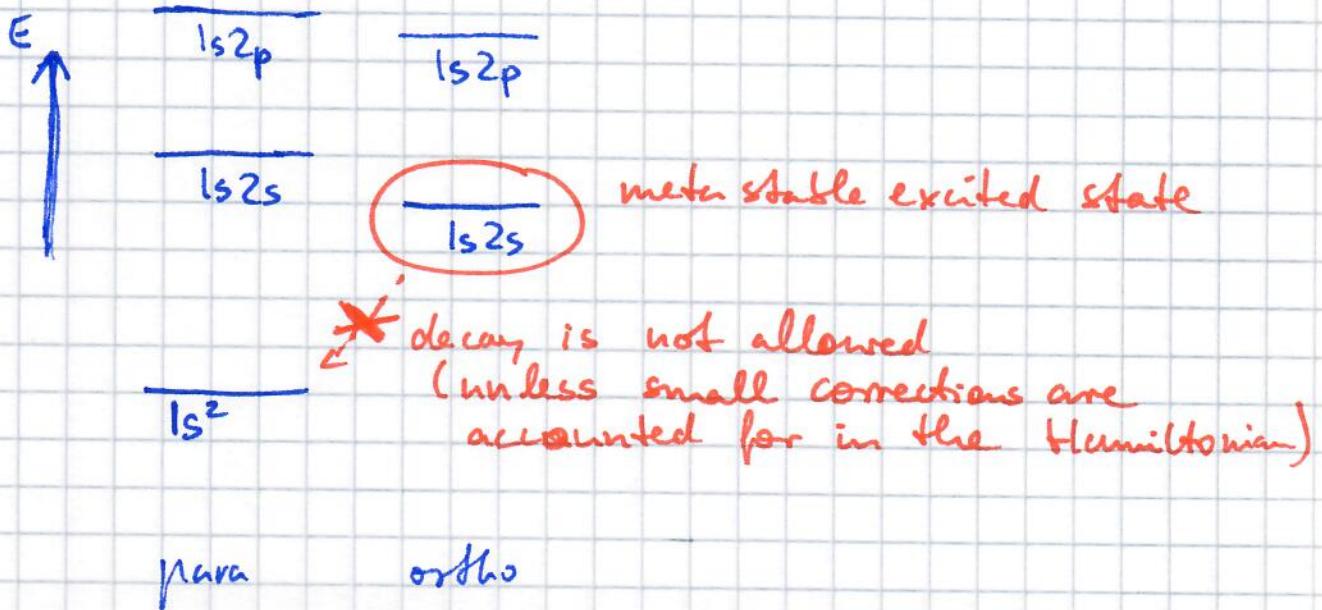
It is readily seen that  $J$  is positive.

So, we have schematically:



Helium spin-singlet states : para-helium

Helium spin-triplet states : ortho-helium



## 7.5 Multi-particle states

We already looked a little bit at  $N$ -particle states.

Let's look at 6 electrons, all in a p-state.

$$\text{p-state} \hat{=} l=1 \Rightarrow m_l = 0, \pm 1$$

$$\text{spin-}\frac{1}{2} \Rightarrow m_s = \pm \frac{1}{2}$$

Can we construct a fully anti-symmetric 6-particle state?

How many permutations?  $6! = 1 \cdot 2 \cdot 3 \cdot 4 \cdot 5 \cdot 6 = 720$

$\Rightarrow$  our wave function will have  
720 terms!!!

Let us assume that the electrons are not interacting. Since  $l=1$  for all 6 electrons and  $s=\frac{1}{2}$ , we just use the "labels" (quantum numbers)  $m_l$  and  $m_s$ .

Thus, we have 6 distinct states:

$$\Psi_{0,\pm\frac{1}{2}}; \Psi_{1,\pm\frac{1}{2}}; \Psi_{-1,\pm\frac{1}{2}}$$

Let's denote the position vectors of the electrons by  $\vec{x}_1, \vec{x}_2, \dots, \vec{x}_6$ .

Then, state  $\varphi_{0,+ \frac{1}{2}}$  can be occupied by the first electron, or the second electron, or the third electron, or ...

→ any of the electrons has  $\frac{1}{6}$  of its probability in state  $m_l=0, m_s=+\frac{1}{2}$ ;  $\frac{1}{6}$  of its probability in state  $m_l=0, m_s=-\frac{1}{2}$ ;  $\frac{1}{6}$  of its probability in state  $m_l=+1, m_s=+\frac{1}{2}$ ; ...

The wave function can be written in the form of a Slater determinant:

$$\frac{1}{\sqrt{6!}} \det \begin{vmatrix} \varphi_{0,\frac{1}{2}}(\vec{x}_1) & \varphi_{0,\frac{1}{2}}(\vec{x}_2) & \varphi_{0,\frac{1}{2}}(\vec{x}_3) & \varphi_{0,\frac{1}{2}}(\vec{x}_4) & \varphi_{0,\frac{1}{2}}(\vec{x}_5) & \varphi_{0,\frac{1}{2}}(\vec{x}_6) \\ \varphi_{0,-\frac{1}{2}}(\vec{x}_1) & \varphi_{0,-\frac{1}{2}}(\vec{x}_2) & \varphi_{0,-\frac{1}{2}}(\vec{x}_3) & \dots & & \\ \varphi_{1,\frac{1}{2}}(\vec{x}_1) & : & \varphi_{1,\frac{1}{2}}(\vec{x}_3) & & & \\ \varphi_{1,-\frac{1}{2}}(\vec{x}_1) & & & \varphi_{1,-\frac{1}{2}}(\vec{x}_4) & & \\ \varphi_{-1,\frac{1}{2}}(\vec{x}_1) & & & & \varphi_{-1,\frac{1}{2}}(\vec{x}_5) & \\ \varphi_{-1,-\frac{1}{2}}(\vec{x}_1) & & & & & \varphi_{-1,-\frac{1}{2}}(\vec{x}_6) \end{vmatrix}$$

$\underbrace{\hspace{20em}}$   
 $6 \times 6$  matrix

## Second quantization

A different way of doing Schrödinger quantum mechanics (particularly well suited for many-body systems).

The name is a bit unfortunate: Nothing gets quantized a second time — it just looks as if it were ...

First quantization: formulation 1 Second quantization: formulation 2	}	same physics → same results
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Let us look at the density in first quantization.

$$\text{Single particle: } n(\vec{x}) = \psi^*(\vec{x}) \psi(\vec{x})$$



wave function and complex conjugate of wave function

$$\int n(\vec{x}) d\vec{x} = 1$$

$$\text{Many particles: } n(\vec{x}_i) = \int \psi^+(\vec{x}_1, \vec{x}_2, \dots, \vec{x}_N) \psi(\vec{x}_1, \vec{x}_2, \dots, \vec{x}_N) d\vec{x}_2 \dots d\vec{x}_N$$


  
 Single-particle  
 density (often just  
 called density)


  
 N-particle wave  
 fct

$$\int n(\vec{x}_i) d\vec{x}_i = N$$

Going to second quantization ( $\equiv$  using alternative formulation):

$$\hat{n}(\vec{x}) = \hat{\psi}^+(\vec{x}) \hat{\psi}(\vec{x})$$


  
 density operator      adjoint      field operator

$\hat{\psi}^+(\vec{x})$ : creates a particle  
at position  $\vec{x}$

$\hat{\psi}(\vec{x})$ : destroys a particle  
at position  $\vec{x}$

$$\hat{N} = \int \hat{\psi}^+(\vec{x}) \hat{\psi}(\vec{x}) d^3x$$


  
 total particle  
 number operator

the field operator looks  
as though we  
quantized the wave  
fct. again - but this  
is not the case!

We know:

If we have more than 1 particle of a given kind, we have to worry about the proper symmetrization (identical bosons) or proper anti-symmetrization (identical fermions).

$\rightarrow$  this is built into the second quantization formalism

(we do not need to do this by hand - we have a "smarter" way of keeping track of the  $N!$  permutations).

Let us introduce states in Fock space:

$\{ |n_1, n_2, \dots, n_N \rangle \}$   $\rightarrow$  these states span the Fock space

number of particles with eigenvalue  $E_1$ , (e.g.) for some operator ( $\hat{=}$  single particle operator)  
 $\rightarrow$  could be kinetic energy operator

number of particles with eigenvalue  $E_2$  for some operator

For example:  $|0, 0, \dots, 0\rangle = |\vec{0}\rangle$  vacuum

(note: vacuum ≠ nothing)

$|1, 0, \dots, 0\rangle$  state with one particle

Let's start with vacuum and let's construct N-particle state from the vacuum. Let's do this step-by-step:

First, create 1-particle state from vacuum state.

Then, create 2-particle state from 1-particle state,  
and so on ...

$|0\rangle$  vacuum

operate with  $\hat{a}_i^+$  to create a particle in a state  
with eigenvalue  $\vec{k}_i$ :

$$\hat{a}_i^+ |0\rangle = |1\rangle$$

Act with  $\hat{a}_i^-$  to destroy the particle in the state with  
eigenvalue  $\vec{k}_i$ :

$$\hat{a}_i^- |1\rangle = |0\rangle$$

More concretely: What do we mean when we say

"in a state w/ eigenvalue  $\vec{k}$ ?"

Plane wave state:  $\hat{a}_p^+ |0\rangle$  creates a particle in plane wave state with momentum  $\vec{p}$ .

Two level system:  $|12\rangle$   
 $|11\rangle$

$\hat{a}_1^+ |0\rangle$  creates a particle in state  $|11\rangle$  of the two-level system.

So far so good: The "trouble" arises when we want to add a second particle.

When we add the second particle, we have to specify whether the two particles are

- identical bosons: bosonic creation / annihilation operators
- identical fermions: fermionic creation / annihilation operators
- distinguishable particles: nothing to worry about (no symmetrization / anti-symmetrization)

Let's deal with bosons first: they are easier since we can place as many identical bosons in the same state as we wish.

For bosons: Say, we already have  $n$  bosons in a

given state  $|n\rangle$ .

$n$  particles in state with eigenvalue  $E_n$ .

Then:

$$\hat{a}_i^+ |n\rangle = \sqrt{n+1} |n+1\rangle \quad \text{particle creation operator}$$

$$\hat{a}_i |n\rangle = \sqrt{n} |n-1\rangle \quad \text{particle annihilation operator}$$

How do we create  $|n\rangle$ ?

$$|n\rangle = \frac{(\hat{a}_i^+)^n}{\sqrt{n!}} |0\rangle$$

Let's see what we get:

$$(\hat{a}_i \hat{a}_i^+ - \hat{a}_i^+ \hat{a}_i) |n\rangle = \hat{a}_i \sqrt{n+1} |n+1\rangle$$

applying the  
rules introduced  
above

$$- \hat{a}_i^+ \sqrt{n} |n-1\rangle$$

$$= [(n+1) - n] |n\rangle$$

$$= |n\rangle$$

$$\Rightarrow \hat{a}_1 \hat{a}_1^\dagger - \hat{a}_1^\dagger \hat{a}_1 = 1$$

$$\text{or } [\hat{a}_1, \hat{a}_1^\dagger] = 1$$

It can be shown easily:  $[\hat{a}_1, \hat{a}_1] = [\hat{a}_1^\dagger, \hat{a}_1^\dagger] = 0$

$$\langle n | \hat{a}_1^\dagger = \sqrt{n} \langle n-1 |$$

✓

acts to left and removes a particle

$$\langle n | \hat{a}_1 = \sqrt{n+1} \langle n+1 |$$

✓

acts to left and creates a particle

$$\hat{a}_1^\dagger \hat{a}_1 |n\rangle = \hat{a}_1^\dagger \sqrt{n} |n-1\rangle = n |n\rangle \Rightarrow \hat{a}_1^\dagger \hat{a}_1 \text{ counts}$$

the # of particles  
in state

Note: instead of subscript 1, we could have used subscript 2.

This means that we can look at more general case (everything carries over):

$$\hat{a}_j^+ | \dots, n_j, \dots \rangle = \sqrt{n_j + 1} | \dots, n_j + 1, \dots \rangle$$

$$\hat{a}_j^- | \dots, n_j, \dots \rangle = \sqrt{n_j} | \dots, n_j - 1, \dots \rangle$$

$$[\hat{a}_i, \hat{a}_j^+] = \delta_{ij}$$

$$[\hat{a}_i^+, \hat{a}_j^+] = [\hat{a}_i, \hat{a}_j^-] = 0 \text{ for all } i, j \text{ combinations}$$

$$[\hat{b}, \hat{c}] = \hat{b}\hat{c} - \hat{c}\hat{b}$$

↑  
definition

For example:  $[\hat{a}_1^+, \hat{a}_2^+] = 0$

$$\Rightarrow \hat{a}_1^+ \hat{a}_2^+ - \hat{a}_2^+ \hat{a}_1^+ = 0$$

$$\Rightarrow \hat{a}_1^+ \hat{a}_2^+ = \hat{a}_2^+ \hat{a}_1^+$$

$$\Rightarrow \underbrace{\hat{a}_1^+ \hat{a}_2^+ |0\rangle}_{|1,1\rangle} = \underbrace{\hat{a}_2^+ \hat{a}_1^+ |0\rangle}_{|1,1\rangle} = 0$$

$$\underbrace{|1,1\rangle}_{\text{under}} = \underbrace{|1,1\rangle}_{\text{over}}$$

It doesn't matter in which order we fill the slots ("democratic"). BOSONS

$$|n_1, n_2\rangle = \frac{(\hat{a}_2^+)^{n_1}}{\sqrt{n_1!}} \frac{(\hat{a}_1^+)^{n_2}}{\sqrt{n_2!}} |0, 0\rangle$$

For identical fermions:

As alluded to earlier, we need to think about anti-symmetrization. We want our formalism to somehow "automatically" build in ( $\equiv$  take care of) anti-symmetrization.

Note: We can have  $|0\rangle$  (no fermion in state with a given eigenvalue) &  $|1\rangle$  (one fermion in state with a given eigenvalue).

We cannot have  $|2\rangle, |3\rangle, \dots$  for identical fermions.

As in the boson case, let's start off with vacuum state and then let's add one fermion to the vacuum state, and then let's add another fermion to the one-fermion state, and so on.

Define:  $\hat{a}_i |0\rangle = 0$     or note: " $0$ " is different from " $|0\rangle$ "

$$\hat{a}_i |1\rangle = |0\rangle$$

$$\hat{a}_i^+ |0\rangle = |1\rangle$$

$$\hat{a}_i^+ |1\rangle = 0 \quad \text{or this guarantees that we cannot put two fermions in the same state}$$

Matrix representation of  $\hat{a}_i$ ?

$$\begin{matrix} & |10\rangle & |11\rangle \\ \langle 01| & \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \\ \langle 11| & \end{matrix}$$

Matrix representation of  $\hat{a}_i^+$ ?

$$\begin{matrix} & |10\rangle & |11\rangle \\ \langle 01| & \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \\ \langle 11| & \end{matrix}$$

Let's look at:

$$(\hat{a}_i \hat{a}_i^+ + \hat{a}_i^+ \hat{a}_i) |10\rangle = \hat{a}_i |11\rangle + 0 = |10\rangle$$

$$(\hat{a}_i \hat{a}_i^+ + \hat{a}_i^+ \hat{a}_i) |11\rangle = 0 + \hat{a}_i^+ |10\rangle = |11\rangle$$

↗  
applying the  
definitions from above

$$\Rightarrow \hat{a}_i \hat{a}_i^+ + \hat{a}_i^+ \hat{a}_i = 1$$

$$\Rightarrow \{\hat{a}_i, \hat{a}_i^+\} = 1 \quad \text{anti-commutation relation}$$

$$\text{Easy to check: } \{\hat{a}_i, \hat{a}_j\} = \{\hat{a}_i^+, \hat{a}_j^+\} = 0$$

As in the boson case, we can write this in general for  $\hat{a}_i$  and  $\hat{a}_j^+$ :

FOR  
FERMIONS

$$\boxed{\begin{aligned} \{\hat{a}_i, \hat{a}_j^+\} &= \delta_{ij} \\ \{\hat{a}_i, \hat{a}_j\} &= \{\hat{a}_i^+, \hat{a}_j^+\} = 0 \quad \text{for all } i, j \text{ combinations} \end{aligned}}$$

$$\{\hat{b}, \hat{c}\} = \hat{b}\hat{c} + \hat{c}\hat{b} \quad \text{anti-commutator}$$

Example:  $\{\hat{a}_1^+, \hat{a}_2^+\} = 0$

$$\Rightarrow \hat{a}_1^+ \hat{a}_2^+ + \hat{a}_2^+ \hat{a}_1^+ = 0$$

$$\Rightarrow \hat{a}_1^+ \hat{a}_2^+ = - \hat{a}_2^+ \hat{a}_1^+$$

$$\Rightarrow \hat{a}_1^+ \hat{a}_2^+ |0\rangle = - \hat{a}_2^+ \hat{a}_1^+ |0\rangle$$

Thus: the order in which we create particles matters.

This ensures the anti-symmetry of the wave fct. under the exchange of two identical particles/fermion.

$$|n_1, n_2, \dots \rangle = \dots (\hat{a}_2^+)^{n_2} \underbrace{(\hat{a}_1^+)^{n_1}}_{\uparrow} |0\rangle$$

the factors of

$\frac{1}{\sqrt{n_j!}}$  have been

dropped (since  $n_j$

is equal to 0 or 1,

they are equal to 1)

we need to act w/  $\hat{a}_1^+$  first ... then with  $\hat{a}_2^+$  ... and so on.

Let's play around a little bit:

We know:  $\hat{a}_p^+ |0, 0, \dots, 0\rangle = |1, 0, \dots, 0\rangle$

$\underbrace{\hspace{10em}}$   
vacuum state

We want to calculate  $\hat{a}_p^+ |0, 1, 0, \dots\rangle$ :

$\underbrace{\hspace{10em}}$

We are no longer acting on the vacuum state ("there's already a fermion in the way").

So: somehow, we want to generate the vacuum state so that we can then act with  $\hat{a}_i^+$ .

How do we create vacuum state?

Take fermions that are already there out of the way.

$$\begin{aligned}\hat{a}_i^+ &= \hat{a}_i^+ \left( \underbrace{\hat{a}_2^+ \hat{a}_2^+}_{\equiv 1} + \hat{a}_2^+ \hat{a}_2^- \right) \\ &= \hat{a}_i^+ \hat{a}_2^+ \hat{a}_2^+ + \underbrace{\hat{a}_i^+ \hat{a}_2^+ \hat{a}_2^-}_{-\hat{a}_2^+ \hat{a}_1^+} \\ &= + \hat{a}_i^+ \hat{a}_2^+ \hat{a}_2^+ - \hat{a}_2^+ \hat{a}_i^+ \hat{a}_2^-\end{aligned}$$

$$\text{So: } \hat{a}_1^+ |0, 1, 0, \dots \rangle = (\hat{a}_1^+ \hat{a}_2 \hat{a}_2^+ - \hat{a}_2^+ \hat{a}_1 \hat{a}_2) |0, 1, \dots \rangle$$

previous  
page

$$= +\hat{a}_1^+ \hat{a}_2 \hat{a}_2^+ |0, 1, 0, \dots \rangle$$

$$- \hat{a}_2^+ \hat{a}_1^+ \hat{a}_2 |0, 1, \dots \rangle$$

$$= 0 - \underbrace{\hat{a}_2^+ \hat{a}_1^+}_{\text{now we have}} \underbrace{\hat{a}_2}_{\hat{a}_1^+ \text{ acting on } |0\rangle} |0, 1, \dots \rangle$$

$\hat{a}_1^+$  acting on  $|0\rangle$   $|0, 0, 0, \dots \rangle$   
and we know what that is

$$= -\hat{a}_2^+ \underbrace{\hat{a}_1^+ \hat{a}_2}_{|1, 0, \dots \rangle} |0, 1, 0, \dots \rangle$$

$$= -|1, 1, 0, \dots \rangle$$

"we always want to start filling from the beginning" !!!

"we always want to start filling from the beginning" !!!

In general:  $\hat{a}_j^+ |n_1, n_2, \dots, n_j, \dots \rangle$

$$\begin{aligned} & \xrightarrow{\substack{\exists j: n_j = 1: 1-n_j = 0 \\ \exists j: n_j = 0: 1-n_j = 1}} = (1-n_j) (-1)^{\sum_{k>j} n_k} |n_1, \dots, n_j+1, \dots \rangle \\ & \hat{a}_j^+ |n_1, \dots, n_j, \dots \rangle \end{aligned}$$

$$\begin{aligned} & \xrightarrow{\substack{\exists j: n_j = 0 \rightarrow = 0 \\ \exists j: n_j = 1 \rightarrow = 1}} = n_j (-1)^{\sum_{k>j} n_k} |n_1, \dots, n_j-1, \dots \rangle \end{aligned}$$

What about the unperturbed spin-singlet state of He-atom?

Let  $\hat{a}_{nlm_s}^+$  be operator that creates electron in state  $\psi_{nlm_s}^{z=2}(\vec{x}) X_{\frac{1}{2}, m_s}$ .

Similarly,  $\hat{a}_{nlm_s}$  destroys electron in state  $\psi_{nlm_s}^{z=2}(\vec{x}) X_{\frac{1}{2}, m_s}$ .

We order our states from lowest to highest:

$$100 - \frac{1}{2} \rightsquigarrow \text{slot 1}$$

$$100 + \frac{1}{2} \rightsquigarrow \text{slot 2}$$

$$200 - \frac{1}{2} \rightsquigarrow \text{slot 3}$$

$$200 + \frac{1}{2}$$

$$21-1-\frac{1}{2}$$

$$21-1+\frac{1}{2}$$

$$210 - \frac{1}{2}$$

$$210 + \frac{1}{2}$$

$$211 - \frac{1}{2}$$

$$211 + \frac{1}{2}$$

Singlet state:  $\hat{a}_{100 \frac{1}{2}}^+ \hat{a}_{100 - \frac{1}{2}}^+ |0\rangle$   
(gr. st.)

We need to agree on an ordering and then use the same ordering throughout the entire calculation.

Triplet state? First s.t. that doesn't work:

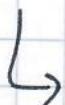
$$\hat{a}_{100\pm}^+ a_{100\pm}^+ |0\rangle = 0$$

follows from commutator

Need to change some g.n.:

$$\hat{a}_{2\ell m_\ell - \frac{1}{2}}^+ \hat{a}_{100 - \frac{1}{2}}^+ |0\rangle$$

(generates triplet  
 $\downarrow \uparrow \downarrow \uparrow$ )



this is equal to

$$-\hat{a}_{100 - \frac{1}{2}}^+ \hat{a}_{2\ell m_\ell - \frac{1}{2}}^+ |0\rangle$$

(by commutator rule)

better: anti-commutator

Let's consider particles in a box with periodic BC:

$$\psi_{\vec{k}}(x) = \frac{1}{L^{3/2}} e^{i\vec{k} \cdot \vec{x}}$$

$\hat{a}_{\vec{k}, ms}^+$  : adds a particle with momentum  $i\vec{k}$   
and spin projection g.n.  $ms$  to the box

$\hat{a}_{\vec{k}, ms}$  : removes ...

The amplitude at the point  $\vec{x}'$  for finding the particle added by  $\hat{a}_{k,m_s}^+$  is

$$\frac{e^{-ik\cdot\vec{x}'}}{L^{3/2}}$$

Let's introduce  $\hat{\psi}_{m_s}^+(\vec{x}) = \sum_{\vec{k}} \underbrace{\frac{e^{-ik\cdot\vec{x}}}{\sqrt{L^3}}}_{\text{adds particle to the system}} \hat{a}_{k,m_s}^+$

adds particle to the system

in a superposition of momentum states with amplitude  $\frac{e^{-ik\cdot\vec{x}}}{L^{3/2}}$

$\hat{\psi}_{m_s}^+(\vec{x})$  adds all the amplitude at  $\vec{x}$ .

$$\hat{\psi}_{m_s}^-(\vec{x}) = \sum_{\vec{k}} \frac{e^{ik\cdot\vec{x}}}{\sqrt{L^3}} \hat{a}_{k,m_s}^- \text{ removes a particle from point } \vec{x}.$$

$\hat{\psi}_{m_s}^+(\vec{x})$  and  $\hat{\psi}_{m_s}^-(\vec{x})$  are field operators.

$$\hat{\psi}^+(\vec{x}) |0\rangle = \sum_{\vec{k}} \underbrace{\frac{e^{-ik\cdot\vec{x}}}{L^{3/2}}}_{\text{forget about spin for a moment}} \underbrace{\hat{a}_{\vec{k}}^+}_{\langle \vec{k} | \vec{x} \rangle} |0\rangle$$

forget about spin for a moment  $\langle \vec{k} | \vec{x} \rangle | \vec{k} \rangle$

$$= \sum_{\vec{k}} \underbrace{| \vec{k} \rangle \langle \vec{k} |}_{\text{completeness}} \vec{x} = | \vec{x} \rangle$$

$\hat{\psi}^+(\vec{x})$  adds particle at  $| \vec{x} \rangle$

We can invert the equations:

$$\hat{\psi}_{m_s}^+(\vec{x}) = \sum_{\vec{k}} \frac{e^{-i\vec{k} \cdot \vec{x}}}{L^{3/2}} \hat{a}_{\vec{k}, m_s}^+$$

$$\Rightarrow \frac{e^{-i\vec{k}' \cdot \vec{x}}}{L^{3/2}} \hat{\psi}_{m_s}^+(\vec{x}) = \sum_{\vec{k}} \frac{e^{-i(\vec{k}-\vec{k}') \cdot \vec{x}}}{(L^{3/2})^2} \hat{a}_{\vec{k}', m_s}^+$$

integrate over  $\int \dots d^3 \vec{x}$ :

$$\hat{a}_{\vec{k}, m_s}^+ = \int \frac{e^{i\vec{k} \cdot \vec{x}}}{L^{3/2}} \hat{\psi}_{m_s}^+(\vec{x}) d^3 \vec{x}$$

Similarly:

$$\hat{a}_{\vec{k}, m_s}^+ = \int \frac{e^{-i\vec{k} \cdot \vec{x}}}{L^{3/2}} \hat{\psi}_{m_s}^+(\vec{x}) d^3 \vec{x}$$

In general:  $\hat{\psi}^+(\vec{x}) = \sum_j \psi_j^*(\vec{x}) \hat{a}_j^+$

$$\hat{\psi}(\vec{x}) = \sum_j \psi_j(\vec{x}) \hat{a}_j$$

where  $\psi_j(\vec{x})$  any single-particle basis

$$\int \psi_j^*(\vec{x}) \psi_i(\vec{x}) d^3 \vec{x} = \delta_{ij}$$

$$\hat{a}_j^+ = \int \varphi_j(\vec{x}) \hat{\psi}^+(\vec{x}) d^3x$$

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$$\hat{a}_j^- = \int \varphi_j^*(\vec{x}) \hat{\psi}^-(\vec{x}) d^3x$$

$\hat{a}_j^+$  creates particle in single-particle state  $\varphi_j(\vec{x})$

(commutator relations:

$$\text{Bosons: } [\hat{\psi}(\vec{x}), \hat{\psi}(\vec{x}')] = 0$$

$$[\hat{\psi}^+(\vec{x}), \hat{\psi}^+(\vec{x}')] = 0$$

$$[\hat{\psi}(\vec{x}), \hat{\psi}^+(\vec{x}')] = \delta(\vec{x} - \vec{x}')$$

$$\text{Fermions: } \{ \hat{\psi}(\vec{x}), \hat{\psi}(\vec{x}') \} = 0$$

$$\{ \hat{\psi}^+(\vec{x}), \hat{\psi}^+(\vec{x}') \} = 0$$

$$\{ \hat{\psi}(\vec{x}), \hat{\psi}^+(\vec{x}') \} = \delta(\vec{x} - \vec{x}')$$

In general, we are dealing with a many-body Hamiltonian of the following form:

$$\hat{H} = \sum_j \hat{T}_j + \sum_j \hat{V}_j + \sum_{j < k} \hat{V}_{jk} + \sum_{j < k < l} \hat{V}_{jkl} + \dots$$

↓                      ↓                      ↓  
 kinetic                single-particle        two-body  
 energy of            potential                interaction  
 $j^{\text{th}}$  particle

Let's write the kinetic energy operator in terms of  $\hat{a}_{\vec{k}}^\dagger$  and  $\hat{a}_{\vec{k}}^\dagger$  operators.

To "measure" the kinetic energy of a system, we count the number of particles with momentum  $t\vec{k}$ , multiply it by  $\frac{t^2 \hbar^2}{2m}$  (i.e., the kinetic energy of a particle with momentum  $t\vec{k}$ ), and then sum over all  $\vec{k}$ :

$$\Rightarrow \hat{T} = \sum \frac{t^2 \hbar^2}{2m} \hat{a}_{\vec{k}}^\dagger \hat{a}_{\vec{k}}$$

here, we are taking advantage of the fact that the eigenkets of the kinetic energy operator are plane waves.

If we consider fermions in different spin states,  
then we have:

$$\hat{T} = \sum_{m_s} \sum_{\vec{k}} \frac{t^2 k^2}{2m} \hat{a}_{\vec{k}, s_m}^+ \hat{a}_{\vec{k}, m_s}^-$$

We had  $\hat{T} = \sum_{\vec{k}} \frac{\hbar^2 \vec{k}^2}{2m} \hat{a}_{\vec{k}}^+ \hat{a}_{\vec{k}}$  ( $N$ -particle kinetic energy operator)

↑  
neglecting spin

Want to rewrite  $\hat{T}$  in terms of field operators:

$$\hat{a}_{\vec{k}}^+ = \frac{1}{\sqrt{V}} \int e^{i\vec{k} \cdot \vec{x}} \hat{\psi}^+(\vec{x}) d^3x$$

$$\hat{a}_{\vec{k}} = \frac{1}{\sqrt{V}} \int e^{-i\vec{k} \cdot \vec{x}'} \hat{\psi}(\vec{x}') d^3x'$$

Plug these definitions / relations into  $\hat{T}$ :

$$\begin{aligned} \hat{T} &= \frac{1}{2m} \frac{1}{V} \sum_{\vec{k}} \iint \underbrace{\hbar^2 \vec{k}^2}_{\substack{\text{split } \hbar^2 \vec{k}^2 \\ \text{into product}}} e^{-i\vec{k} \cdot \vec{x}} \cdot \underbrace{\hbar^2 \vec{k}^2}_{\substack{\text{split } \hbar^2 \vec{k}^2 \\ \text{into product}}} e^{-i\vec{k} \cdot \vec{x}'} \hat{\psi}^+(\vec{x}) \hat{\psi}(\vec{x}') \\ &\quad -i\hbar \vec{\nabla}_{\vec{x}} e^{i\vec{k} \cdot \vec{x}} \quad i\hbar \vec{\nabla}_{\vec{x}'} e^{-i\vec{k} \cdot \vec{x}'} \end{aligned}$$

$$= \frac{\hbar^2}{2m} \frac{1}{V} \sum_{\vec{k}} \iint (\vec{\nabla}_{\vec{x}} e^{i\vec{k} \cdot \vec{x}}) \cdot (\vec{\nabla}_{\vec{x}'} e^{-i\vec{k} \cdot \vec{x}'}) \hat{\psi}^+(\vec{x}) \hat{\psi}(\vec{x}')$$

Separate  $\vec{x}$  and  $\vec{x}'$  parts

$$= \frac{\hbar^2}{2m} \frac{1}{V} \sum_{\vec{k}} \int (\vec{\nabla}_{\vec{x}} e^{i\vec{k} \cdot \vec{x}}) \hat{\psi}^+(\vec{x}) d^3x \cdot \int (\vec{\nabla}_{\vec{x}'} e^{-i\vec{k} \cdot \vec{x}'}) \hat{\psi}(\vec{x}') d^3x'$$

$$= \frac{\hbar^2}{2m} \sum_i \left( \int e^{-i\vec{k} \cdot \vec{x}} \vec{\nabla}_{\vec{x}} \hat{\psi}^+(\vec{x}) d^3x \right) \cdot \left( \int e^{-i\vec{k} \cdot \vec{x}'} \vec{\nabla}_{\vec{x}'} \hat{\psi}(\vec{x}') d^3x' \right)^T \quad 7-44$$

integrating by  
parts for both  
integrals (surface term  
assumed to vanish)

$$\text{"recombining"} = \frac{\hbar^2}{2m} \iint \sum_i \frac{1}{\hbar} \underbrace{e^{i\vec{k} \cdot \vec{x}} e^{-i\vec{k} \cdot \vec{x}'} (\vec{\nabla}_{\vec{x}} \hat{\psi}^+(\vec{x})) \cdot (\vec{\nabla}_{\vec{x}'} \hat{\psi}(\vec{x}'))}_{{\delta}(\vec{x} - \vec{x}')} d^3x d^3x'$$

$$\text{use S-fct.} \rightarrow = \frac{\hbar^2}{2m} \int (\vec{\nabla}_{\vec{x}} \hat{\psi}^+(\vec{x})) \cdot (\vec{\nabla} \hat{\psi}(\vec{x})) d^3x$$

to "collapse"  
integrals

$$\text{So: } \boxed{\hat{T} = \frac{\hbar^2}{2m} \int (\vec{\nabla}_{\vec{x}} \hat{\psi}^+(\vec{x})) \cdot (\vec{\nabla} \hat{\psi}(\vec{x})) d^3x}$$

no sum over the number  
of particles (despite of the  
fact that this is the many-  
body kinetic energy operator)

In general: If  $\hat{H} = \sum_{j=1}^N \hat{h}_j$ , then  
 $\underbrace{\hat{h}_j}_{\text{single-particle operator}}$

$$\hat{H} = \int \hat{\psi}^+(\vec{x}) \hat{h} \hat{\psi}(\vec{x}) d^3x.$$

$$\text{In particular: } \hat{h}_j = \hat{T}_j$$

$$\Rightarrow \hat{H} = \int \hat{\psi}^+(\vec{x}) \frac{-\hbar^2}{2m} \vec{\nabla}_{\vec{x}}^2 \hat{\psi}(\vec{x}) d^3x.$$

So far, we have dealt with <sup>sum</sup> over single-particle terms in the many-body Hamiltonian. In general, the Hamiltonian will contain a sum over two-body potentials or maybe even three-body terms. We need to learn how to write Hamiltonian that contains two-body terms in 2<sup>nd</sup> quantization.

$$\text{Let } \hat{V}^{(2)} = \sum_{\alpha < \beta} f^{(2)}(\vec{x}_\alpha, \vec{x}_\beta)$$



could be a ~~two~~-body potential

We want to rewrite this in terms of  $\hat{a}$  and  $\hat{a}^\dagger$  as well as in terms of  $\hat{\psi}^+(\vec{x})$  and  $\hat{\psi}(\vec{x})$ .

To do this, we will need to proof an auxiliary identity:

$$\boxed{\sum_{\alpha=1}^N |\psi_i>_\alpha \langle \psi_j| = \hat{a}_i^\dagger \hat{a}_j}$$

Proof: ↗ will be done on page 7-49

We will start with the Fock state and write it out formally in terms of the single particle states (we have been avoiding that up to now):

$$\langle \vec{x} | \dots, n_i, \dots, n_j, \dots \rangle = \frac{1}{N!} \sum_{\text{P}} \underbrace{\varphi_i(\vec{x}_{i+1}) \varphi_i(\vec{x}_{i+2}) \dots \varphi_i(\vec{x}_{i+n_i})}_{\varphi_i \text{ appears } n_i \text{ times}} \cdot \underbrace{\dots \varphi_j(\vec{x}_{j+n_j}) \varphi_j(\vec{x}_{j+n_j+1}) \dots \varphi_j(\vec{x}_{j+n_j+n_j})}_{\varphi_j \text{ appears } n_j \text{ times}} \cdot \frac{1}{\sqrt{n_1!}} \frac{1}{\sqrt{n_2!}} \dots \frac{1}{\sqrt{n_i!}} \dots \frac{1}{\sqrt{n_j!}} \dots$$

stands for  
all the position  
vectors:  
 $\vec{x}_1, \dots, \vec{x}_N$

Sum over  
all permutations  
( $N!$  terms)

Say  $N=2$  and  $n_i=2$ :

$$\langle \vec{x}_1, \vec{x}_2 | z \rangle = \frac{1}{2!} \sum_{\text{P}} \underbrace{\varphi_i(\vec{x}_1) \varphi_i(\vec{x}_2)}_{\varphi_i(\vec{x}_1) \varphi_i(\vec{x}_2) + \varphi_i(\vec{x}_2) \varphi_i(\vec{x}_1)} \frac{1}{\sqrt{2!}}$$

$$\underbrace{\varphi_i(\vec{x}_1) \varphi_i(\vec{x}_2) + \varphi_i(\vec{x}_2) \varphi_i(\vec{x}_1)}_{2! \text{ permutations}}$$

$$= \varphi_i(\vec{x}_1) \varphi_i(\vec{x}_2)$$

fully symmetrized state

Multiply green eq. w/  $\varphi_j^*(\vec{x}_a)$  and integrate over  $d^3\vec{x}_a$ :

$$\Rightarrow \int \varphi_j^*(\vec{x}_a) \varphi_i(\vec{x}_1, \dots, n_i, \dots, n_j, \dots) d^3\vec{x}_a$$

$$= \frac{1}{N!} \frac{1}{P!} \sum \int \varphi_i(\vec{x}_{k+1}) \cdots \varphi_i(\vec{x}_{k+n_i})$$

$\nearrow$   
 $n_i$  non-zero  
d-terms

$$\cdots \varphi_j^*(\vec{x}_a) \varphi_i(\vec{x}_{k+1}) \cdots \varphi_i(\vec{x}_{k+n_j}) d^3\vec{x}_a$$

$$\cdot \frac{1}{n_1!} \cdots \frac{1}{n_i!} \cdots \frac{1}{n_j!} \cdots$$

get a  $\delta$ -fct. when  
 $\vec{x}_a$  is equal to  
 a specific  $\vec{x}_m \rightarrow$   
 but that specific  
 $\vec{x}_m$  sits in any  
 of the orbitals

due to the permutations  
 $\rightarrow$  we get  $n_j$  Kronecker  
 $\delta$ -fcts.

and sum over  $a$

Next, we multiply by  $\varphi_i(\vec{x}_a)$ . Effectively, this means that we now have a  $\varphi_i(\vec{x}_a)$  where we used to have a  $\varphi_j(\vec{x}_a)$ .

So: The occupation number of  $n_j$  gets lowered by one and the occupation number of  $n_i$  gets increased by one.

Let's write it out:

$$\sum_{\vec{x}} \varphi_i(\vec{x}_\alpha) \int \varphi_j^*(\vec{x}_\alpha) \delta_{n_1, \dots, n_i, \dots, n_j, \dots} d^3 \vec{x}_\alpha$$

$$= \sum_{\alpha} \frac{1}{\sqrt{n!}} \cdot \frac{1}{\sqrt{n_1!}} \cdot \dots \cdot \frac{1}{\sqrt{n_i!}} \cdot \dots \cdot \frac{1}{\sqrt{n_j!}} \cdot \dots$$

$$\sum_{\vec{\Omega}} \int \varphi_i(\vec{x}_\alpha) \varphi_i(\vec{x}_{\alpha+1}) \dots \varphi_i(\vec{x}_{\alpha+n_i})$$

$$\dots \varphi_j^*(\vec{x}_\alpha) \varphi_j(\vec{x}_{\alpha+1}) \dots \varphi_j(\vec{x}_{\alpha+n_j}) d^3 \vec{x}_\alpha$$

$$= \sum_{\alpha} \frac{1}{\sqrt{n!}} \cdot \frac{1}{\sqrt{n_1!}} \cdot \dots \cdot \frac{1}{\sqrt{n_i!}} \cdot \dots \cdot \frac{1}{\sqrt{n_j!}} \cdot \dots \cdot n_j$$

$$\sum_{\vec{\Omega}} \varphi_i(\vec{x}_\alpha) \varphi_i(\vec{x}_{\alpha+1}) \dots \varphi_i(\vec{x}_{\alpha+n_i})$$

$$\dots \varphi_j(\vec{x}_{\alpha+1}) \dots \varphi_j(\vec{x}_{\alpha+n_j-1})$$

$$= \left( \frac{1}{\sqrt{n!}} \cdot \frac{1}{\sqrt{n_1!}} \cdot \dots \cdot \frac{1}{\sqrt{(n_i+1)!}} \cdot \dots \cdot \frac{1}{\sqrt{(n_j-1)!}} \cdot \dots \right)$$

$= \dots, n_i+1, \dots, n_j-1, \dots$

$$\sum_{\vec{\Omega}} \varphi_i(\vec{x}_{\alpha+1}) \dots \varphi_i(\vec{x}_{\alpha+n_i+1}) \dots \varphi_j(\vec{x}_{\alpha+1}) \dots \varphi_j(\vec{x}_{\alpha+n_j-1})$$

$$\left( \cdot n_j \sqrt{(n_i+1)!} \sqrt{(n_j-1)!} \frac{1}{\sqrt{n_i!}} \frac{1}{\sqrt{n_j!}} \right) = \sqrt{n_i+1} \sqrt{n_j}$$

$$\text{So: } \sum_{\alpha} \varphi_i(\vec{x}_{\alpha}) \int \varphi_j^*(\vec{x}_{\alpha}) d^3 \vec{x}_{\alpha} \xrightarrow{n_i, \dots, n_j, \dots} d^3 \vec{x}_{\alpha}$$

$$= \underbrace{\sqrt{n_i+1} \sqrt{n_j} \langle \vec{x} | \dots, n_i+1, \dots, n_j-1, \dots \rangle}_{\langle \vec{x} | \hat{a}_i^+ \hat{a}_j^- | \dots, n_i, \dots, n_j, \dots \rangle}$$

$$\langle \vec{x} | \hat{a}_i^+ \hat{a}_j^- | \dots, n_i, \dots, n_j, \dots \rangle$$

Look at l.h.s.:

$$\underbrace{\sum_{\alpha} \varphi_i(\vec{x}_{\alpha}) \langle \varphi_j |}_{\langle \vec{x}_{\alpha} | \varphi_i \rangle} \underbrace{\int d^3 \vec{x}_{\alpha} \langle \vec{x}_{\alpha} |}_{=1} \langle \tilde{\vec{x}} | \dots, n_i, \dots, n_j \rangle$$

↑  
all  $\vec{x}$ , except  
for  $\vec{x}_{\alpha}$

$$= \sum_{\alpha} |\varphi_i\rangle_{\alpha} \langle \varphi_j | \langle \vec{x} | \dots, n_i, \dots, n_j, \dots \rangle$$

Compare l.h.s.

and r.h.s.  $\Rightarrow$

$$\sum_{\alpha} |\varphi_i\rangle_{\alpha} \langle \varphi_j | = \hat{a}_i^+ \hat{a}_j^-$$

This is the end of the proof!!!

Recall: Our task is to find an expression for

$$V^{(2)} = \sum_{\alpha < \beta} f^{(2)}(\vec{x}_\alpha, \vec{x}_\beta).$$

Step 1 (trivial):

$$V^{(2)} = \frac{1}{2} \sum_{\alpha, \beta} f^{(2)}(\vec{x}_\alpha, \vec{x}_\beta) - \frac{1}{2} \sum_\alpha f^{(2)}(\vec{x}_\alpha, \vec{x}_\alpha)$$

Step 2: Insert closure relations

$$\sum_i |\varphi_i >_\alpha \varphi_i | = 1$$

$$\sum_\delta |\varphi_\delta >_\beta \varphi_\delta | = 1$$

$$\sum_k |\varphi_k >_\alpha \varphi_k | = 1$$

$$\sum_\ell |\varphi_\ell >_\beta \varphi_\ell | = 1$$

$$\Rightarrow \hat{f}^{(2)} = (\underbrace{\sum_i \dots}_{\text{closure relation} = 1})(\underbrace{\sum_\delta \dots}_{=1})(\underbrace{\sum_k \dots}_{=1})(\underbrace{\sum_\ell \dots}_{=1}) \hat{f}^{(2)}$$

$$= \sum_{ij\ell k} \left( |\varphi_i >_\alpha \varphi_i | \right) \left( |\varphi_j >_\beta \varphi_j | \right) \underbrace{|\varphi_k | \varphi_\ell | f^{(2)} | \varphi_k >_\alpha \varphi_\ell |}_{\text{for local operator}}$$

$$\iint \varphi_i^*(\vec{x}_\alpha) \varphi_j^*(\vec{x}_\beta) f^{(2)}(\vec{x}_\alpha, \vec{x}_\beta) \varphi_k(\vec{x}) \varphi_\ell(\vec{x}_\alpha)$$

$$d^3 \vec{x} d^3 \vec{x}$$

$$\text{define: } f_{ijkl}^{(2)} = \int \psi_i^*(\vec{x}_a) \psi_j^*(\vec{x}_b) f^{(2)}(\vec{x}_a, \vec{x}_b)$$

$$\psi_i(\vec{x}_a) \psi_j(\vec{x}_b) d^3 \vec{x}_a d^3 \vec{x}_b$$

$$\Rightarrow \sum_{\alpha \beta} \hat{f}^{(2)} = \sum_{ijkl} \hat{a}_i^+ \underbrace{\hat{a}_k^+ \hat{a}_j^+}_{\hat{a}_j^+ \hat{a}_k^+ + \delta_{kj}} \hat{a}_e \hat{f}_{ijkl}^{(2)}$$

$$\sum_{\alpha} \hat{f}^{(2)} = \sum_{ijkl} \hat{a}_i^+ \hat{a}_k^- \delta_{kj} \hat{f}_{ijkl}^{(2)}$$

$$\Rightarrow \boxed{\hat{V}^{(2)} = \frac{1}{2} \sum_{ijkl} \hat{a}_i^+ \hat{a}_j^+ \hat{a}_k^- \hat{a}_e \hat{f}_{ijkl}^{(2)}}$$

Using field operators:

$$\boxed{\hat{V}^{(2)} = \frac{1}{2} \int \hat{\psi}^+(\vec{x}) \hat{\psi}^+(\vec{x}') \hat{f}^{(2)}(\vec{x}, \vec{x}') \hat{\psi}(\vec{x}') \hat{\psi}(\vec{x}) d^3 \vec{x} d^3 \vec{x}'}$$

Let's look at an example using plane wave basis:

$$\text{Let } \hat{V}^{(1)} = \sum_{\vec{k}} \hat{f}^{(1)}$$

$$\Rightarrow \hat{V}^{(1)} = \sum_{\vec{k}, \vec{k}'} f^{(1)}_{\vec{k}' \vec{k}} \hat{a}_{\vec{k}'}^+ \hat{a}_{\vec{k}}$$

kin. en. op.  
is diagonal in  
plane wave basis  
→ that's why we  
had a single sum

$$\text{where } f^{(1)}_{\vec{k}', \vec{k}} = \int \psi_{\vec{k}'}^*(\vec{x}) f^{(1)}(\vec{x}) \psi_{\vec{k}}(\vec{x}) d^3x$$

$$\left. \begin{array}{c} \frac{1}{\sqrt{v}} e^{-i \vec{k}' \cdot \vec{x}} \\ \left. \begin{array}{c} \frac{1}{\sqrt{v}} e^{-i \vec{k} \cdot \vec{x}} \end{array} \right. \end{array} \right\}$$

$$= \sum_{\vec{k}' \vec{k}} \frac{1}{\sqrt{v}} \int f^{(1)}(\vec{x}) e^{-i (\vec{k}' - \vec{k}) \cdot \vec{x}} d^3x \hat{a}_{\vec{k}'}^+ \hat{a}_{\vec{k}}$$

Fourier transform of single-particle

$$\text{term } f^{(1)} : \hat{f}^{(1)}_{\vec{k}' - \vec{k}}$$

Next: Two-body term  $\hat{V}^{(2)}$

$$\hat{V}^{(2)} = \sum_{\alpha < \beta} \hat{f}^{(2)}_{\alpha \beta}$$

$$V^{(2)} = \sum_{\alpha < \beta} f^{(2)} \underbrace{(\vec{x}_\alpha - \vec{x}_\beta)}$$

we are going to assume dependence

Part of  $\hat{V}^{(2)}$ :

$$\frac{1}{2V^2} \iint e^{-i\vec{k}_1' \cdot \vec{x}_1} e^{-i\vec{k}_2' \cdot \vec{x}_2} f^{(2)}(\vec{x}_1, \vec{x}_2) e^{i\vec{k}_1 \cdot \vec{x}_1} e^{i\vec{k}_2 \cdot \vec{x}_2} d\vec{x}_1 d\vec{x}_2$$

$$\hat{a}_{\vec{k}_1}^\dagger \hat{a}_{\vec{k}_1}^\dagger \hat{a}_{\vec{k}_2}^\dagger \hat{a}_{\vec{k}_2}^\dagger$$

above:  $\bar{f}_{\vec{q}}^{(1)} = \int f^{(1)}(\vec{x}) e^{-i\vec{q} \cdot \vec{x}} d^3 \vec{x}$

$$\Rightarrow f^{(1)}(\vec{x}) = \frac{1}{V} \sum_{\vec{q}} \bar{f}_{\vec{q}}^{(1)} e^{i\vec{q} \cdot \vec{x}}$$

$\xrightarrow{\text{rewrite } f^{(2)} \text{ as a sum over } \vec{q}}$

$$= \frac{1}{2V^3} \sum_{\vec{q}} \bar{f}_{\vec{q}}^{(2)} \iint e^{-i\vec{k}_1' \cdot \vec{x}_1} e^{-i\vec{k}_2' \cdot \vec{x}_2} e^{i\vec{q} \cdot \vec{x}} e^{i\vec{k}_1 \cdot \vec{x}_1} e^{i\vec{k}_2 \cdot \vec{x}_2} d^3 \vec{x}_1 d^3 \vec{x}_2 \hat{a}_{\vec{k}_1}^\dagger \hat{a}_{\vec{k}_1}^\dagger \hat{a}_{\vec{k}_2}^\dagger \hat{a}_{\vec{k}_2}^\dagger$$

$$\vec{x} = \vec{x}_1 - \vec{x}_2$$

$$= \frac{1}{2V} \sum_{\vec{q}} \bar{f}_{\vec{q}}^{(2)} \underbrace{\frac{1}{V} \int e^{-i(\vec{k}_1' - \vec{q} - \vec{k}_1) \cdot \vec{x}_1} d^3 \vec{x}_1}_{\delta_{\vec{k}_1' - \vec{q} - \vec{k}_1, 0}}$$

$$\times \underbrace{\frac{1}{V} \int e^{-i(\vec{k}_2' + \vec{q} - \vec{k}_2) \cdot \vec{x}_2} d^3 \vec{x}_2}_{\delta_{\vec{k}_2' + \vec{q} - \vec{k}_2, 0}} \hat{a}_{\vec{k}_1}^\dagger \hat{a}_{\vec{k}_1}^\dagger \hat{a}_{\vec{k}_2}^\dagger \hat{a}_{\vec{k}_2}^\dagger$$

$$\Rightarrow \frac{1}{2V} \sum_{\vec{q}} \bar{f}_{\vec{q}}^{(2)} \delta_{\vec{k}_1 - \vec{q}, \vec{k}_1} \delta_{\vec{k}_2 + \vec{q}, \vec{k}_2} \hat{a}_{\vec{k}_1}^+ \hat{a}_{\vec{k}_1}^+ \hat{a}_{\vec{k}_2}^- \hat{a}_{\vec{k}_2}^-$$

$$\Rightarrow \hat{V}^{(2)} = \frac{1}{2V} \sum_{\vec{k}_1, \vec{k}_2, \vec{k}_1', \vec{k}_2'} \sum_{\vec{q}} \bar{f}_{\vec{q}}^{(2)} \delta_{\vec{k}_1 - \vec{q}, \vec{k}_1} \delta_{\vec{k}_2 + \vec{q}, \vec{k}_2} \hat{a}_{\vec{k}_1'}^+ \hat{a}_{\vec{k}_1'}^+ \hat{a}_{\vec{k}_2'}^- \hat{a}_{\vec{k}_2'}^-$$

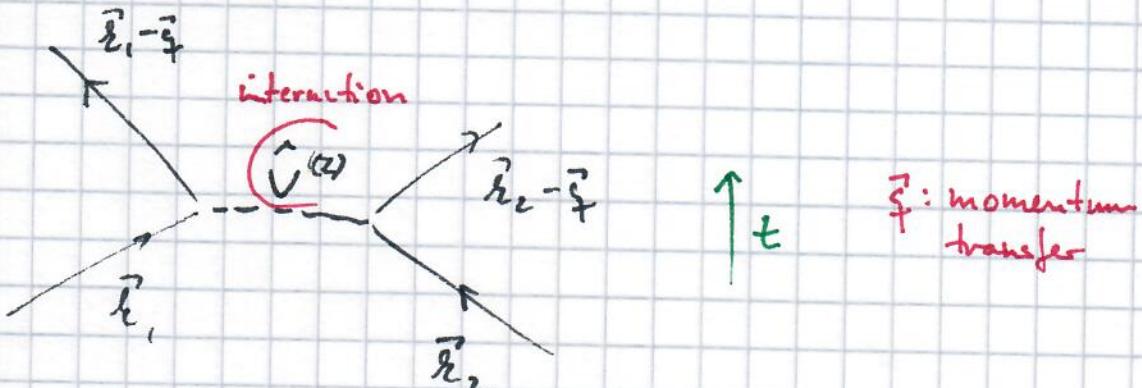
$$= \frac{1}{2V} \sum_{\vec{k}_1, \vec{k}_2, \vec{q}} \bar{f}_{\vec{q}}^{(2)} \hat{a}_{\vec{k}_1 + \vec{q}}^+ \hat{a}_{\vec{k}_2 - \vec{q}}^+ \hat{a}_{\vec{k}_1}^- \hat{a}_{\vec{k}_2}^-$$

only three sums  
because the total  
momentum is conserved

weight factor that  
depends on momentum transfer (FT can  
be readily calculated)

$\vec{k}_1 - \vec{q}$ ,  $\vec{k}_2 + \vec{q}$ :  
outgoing

$\vec{k}_1, \vec{k}_2$ :  
incoming



process is due to  $f^{(2)}$  —  
transition amplitude is  
proportional to  $\bar{f}_{\vec{q}}^{(2)}$

particles w/ momenta  
 $\vec{p}_1$  and  $\vec{p}_2$  get destroyed;  
particles w/ momenta  
 $\vec{p}_1 + t\vec{q}$  and  $\vec{p}_2 - t\vec{q}$   
get created

Non-interacting fermions w/ spin- $\frac{1}{2}$ ,  $G = \uparrow, \downarrow$ :

Ground state:  $|\phi_0\rangle = \prod_{|\vec{k}| < k_F} \prod_{\uparrow, \downarrow} \hat{a}_{\vec{k}G}^+ |0\rangle$

Expectation value of  $\hat{a}_{\vec{k}G}^+ \hat{a}_{\vec{k}G}$ :

$$n_{\vec{k}G} = \langle \phi_0 | \hat{a}_{\vec{k}G}^+ \hat{a}_{\vec{k}G} | \phi_0 \rangle = \begin{cases} 0 & \text{for } |\vec{k}| > k_F \\ 1 & \text{for } |\vec{k}| < k_F \end{cases}$$

Total # of particles  $N$ :

$$N = \sum_{\vec{k}G} n_{\vec{k}G} = 2 \sum_{|\vec{k}| < k_F} = 2 \left(\frac{V}{(2\pi)^3}\right) \int_0^{2\pi} \int_0^{\pi} \int_0^{2\pi} k^2 dk d\theta d\phi$$

from r, l

$$k_x = 2\pi \frac{n_x}{L_x} \Rightarrow dk_x = \frac{2\pi}{L_x} dn_x$$

$$d\vec{k} = \sqrt{\frac{1}{(2\pi)^3}} d^3 \vec{k}$$

$$= \frac{2V}{8\pi^3} 4\pi \frac{1}{3} k_F^3$$

$$= \frac{k_F^3}{3\pi^2} V = \frac{N}{n} \frac{k_F^3}{3\pi^2}$$

↑

$$n = \frac{N}{V} \text{ mean density}$$

$$\Rightarrow h_F^3 = 3\pi^2 n$$

$$\epsilon_F = \frac{\hbar^2 k_F^2}{2m} = \frac{\hbar^2}{2m} (3\pi^2 n)^{2/3}$$

What about  $\langle n(\vec{x}) \rangle$ ?

$$\langle n(\vec{x}) \rangle = \sum_{\zeta} \langle \phi_0 | \hat{\Psi}_{\zeta}^+ (\vec{x}) \hat{\Psi}_{\zeta} (\vec{x}) | \phi_0 \rangle$$

$$\hat{\Psi}^+(\vec{x}) = \sum_{\vec{k}} \phi_{\vec{k}}^*(\vec{x}) \hat{a}_{\vec{k}\zeta}^+$$

$$= \sum_{\zeta} \sum_{\vec{k}} \sum_{\vec{k}'} \frac{e^{-i(\vec{k} \cdot \vec{x} - \vec{k}' \cdot \vec{x})}}{V} \underbrace{\langle \phi_0 | \hat{a}_{\vec{k}\zeta}^+ \hat{a}_{\vec{k}'\zeta}^- | \phi_0 \rangle}_{n_{\vec{k}\zeta} \delta_{\vec{k}\vec{k}'}}$$

$$= \frac{1}{V} \underbrace{\sum_{\zeta} \sum_{\vec{k}} n_{\vec{k}\zeta}}_N$$

$$= \frac{N}{V}$$

$$= n \quad \text{ok: this is what we expected!}$$