

### III. 4 Second quantisation

(105)

- Second quantisation is a formalism that allows to construct in a rather elegant way fully (anti)symmetric many-body states of (fermions) bosons.
- It moreover delivers a general representation of operators in terms of creation and annihilation operators.
- It is based on the description of bosonic and fermionic wave functions in terms of number states.
- To begin the discussion we consider a single mode (state, orbital) that can be populated by bosonic or fermionic particles.
- The state in which no particle is occupying this mode is the vacuum state  $|0\rangle$ , which is normalised:  $\langle 0|0\rangle = 1$ .
- We know that in the case of bosons, the mode can be populated by an arbitrary number of particles, and the state in which the mode is occupied by  $N$  particles is denoted by  $|N\rangle$  (= number state).

Following the discussion of the quantisation of the radiation field, we now introduce bosonic creation ( $a^\dagger$ ) and annihilation ( $a$ ) operators, whose commutator is (106)

$$[a, a^\dagger] = 1.$$

When acting on the number state, they obey

$$a|N\rangle = \sqrt{N}|N-1\rangle$$

$$a^\dagger|N\rangle = \sqrt{N+1}|N+1\rangle,$$

which is consistent with the commutator:

$$[a, a^\dagger]|N\rangle = (a a^\dagger - a^\dagger a)|N\rangle = ((\sqrt{N+1})^2 - (\sqrt{N})^2)|N\rangle = |N\rangle.$$

The number state  $|N\rangle$  can be constructed from the vacuum according to:

$$|N\rangle = \frac{(a^\dagger)^N}{\sqrt{N!}}|0\rangle$$

Moreover, the application of the annihilation operator to the vacuum yields

$$a|0\rangle = 0 \leftarrow \text{zero-``vector''}$$

Let us now discuss the case of fermions.

The difference compared to bosons is that there are only two available states:

Vacuum  $|0\rangle$ , single fermion  $|1\rangle$

- Applying the creation and annihilation operators to both we find:

$$a|0\rangle = 0$$

$$a|1\rangle = |0\rangle$$

$$a^+|0\rangle = |1\rangle$$

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

application of creation operator on already occupied mode does not create a physical state

- We can deduce from these expressions, that  $a^2 = 0$ ,  $a^{+2} = 0$ .

- Moreover, we find that

$$(aa^+ + a^+a)|1\rangle = 0 + |1\rangle = |1\rangle$$

$$(aa^+ + a^+a)|0\rangle = |0\rangle + 0 = |0\rangle,$$

and therefore

$$\underbrace{\{a, a^+\}}_{\text{anticommutator}} = aa^+ + a^+a = 1.$$

anticommutator

Summarising these results yields:

bosons:  $[a, a^+] = 1$ ,  $[a, a] = [a^+, a^+] = 0$

fermions:  $\{a, a^+\} = 1$ ,  $\{a, a\} = \{a^+, a^+\} = 0$

In both cases the number operator is  $a^+a$ :

$$a^+a|N\rangle = N|N\rangle.$$

- We will now generalise these considerations to many modes.
- We begin with bosons and write the fully symmetrised many-body state of  $N$  particles as (using Dirac notation), (108)

$$|4^B\rangle = \frac{1}{N! N_{n_1}! \dots N_{n_N}!} \sum_P |n_1\rangle_{P(1)} \dots |n_N\rangle_{P(N)}$$

- Here we have used the single-body states

$|n_i\rangle$  ↓ quantum number of the single particle state  
j ← label of the particle

- The numbers  $N_{n_i}$  specify how many particles occupy the single-body state with quantum number  $n_i$ .
- As an example consider a state of  $N=18$  bosons, where 5 are in state  $|1\rangle$ , 4 in state  $|4\rangle$  and 9 in state  $|12\rangle$ :

$$|4^B\rangle' = \frac{1}{18! 5! 4! 9!} \sum_P |1\rangle_{P(1)} |1\rangle_{P(2)} |4\rangle_{P(3)} |4\rangle_{P(4)} |12\rangle_{P(5)} |12\rangle_{P(6)} \dots |12\rangle_{P(10)} |12\rangle_{P(11)} |12\rangle_{P(12)} \dots |12\rangle_{P(18)}$$

- This state is fully determined by the occupation numbers 5, 4 and 9, and the other occupation numbers being zero.
- We can therefore write it also as

$$|4_B\rangle' = |5, 0, 0, 4, 0, 0, 0, 0, 0, 0, 0, 9, 0, \dots \rangle$$

- Generally, this leads to the occupation number representation:

$$|N\rangle = |N_1, \dots, N_n, \dots\rangle, \quad N = \sum_k N_k$$

↑                      ↑  
 number of          number  
 particles        of particles  
 in  $|1\rangle$             in  $|n\rangle$

- These states obey the orthogonality relation

$$\langle N'_1, N'_2 \dots | N_1, N_2 \dots \rangle = \delta_{N'_1 N'_1} \delta_{N'_2 N'_2} \dots$$

and the vacuum state is

$$|0\rangle = |0, 0, \dots, 0, \dots\rangle.$$

- These states live in a Hilbert space, which is the tensor product of  $N$  single body Hilbert spaces, where all states are symmetrized:  $\mathcal{H}_N^{\text{sym}} = \mathcal{H} \otimes \mathcal{H} \otimes \dots \otimes \mathcal{H}$ .

- Example:

$$|4\rangle'' = \frac{1}{\sqrt{6}} (|0,0,1,1,0,\dots\rangle - |0,0,2,0,0,\dots\rangle + 2|1,2,0,0,0,0,\dots\rangle)$$

$$= \frac{1}{\sqrt{6}} \left( \frac{1}{\sqrt{2}} (|3\rangle|4\rangle_2 + |4\rangle|3\rangle_2) - |3\rangle|3\rangle_2 + 2|1\rangle|1\rangle_2 \right)$$

- Also, note that

$$\underbrace{|1,1,0,\dots\rangle}_{\text{two particle state}} \neq \underbrace{|1,0,0,\dots\rangle + |0,1,0,\dots\rangle}_{\text{single particle state}}$$

- The particle number representation can be also extended to arbitrary  $N$ , which introduces the so-called Fock-space.

- This space can be written as a direct sum of all Hilbert spaces  $\mathcal{H}_N^{\text{sym}}$ .

$$\mathcal{F}^{\text{sym}} = \mathcal{H}_0^{\text{sym}} \oplus \mathcal{H}_1^{\text{sym}} \oplus \mathcal{H}_2^{\text{sym}} \oplus \dots$$

- These Hilbert spaces are spanned by the following bases:

$$\mathcal{H}_0^{\text{sym}} : |0, 0, \dots\rangle$$

$$\mathcal{H}_1^{\text{sym}} : |1, 0, 0, \dots\rangle, |0, 1, 0, \dots\rangle \dots$$

$$\mathcal{H}_2^{\text{sym}} : |2, 0, 0, \dots\rangle, |0, 2, 0, \dots\rangle \dots$$

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

- For fermions the construction of the particle number states follows a similar procedure.

- We write

$$|\Psi^F\rangle = \frac{1}{N!} \sum_p (-1)^{\pi_p} |n_1\rangle_{p(1)} \dots |n_N\rangle_{p(N)}$$

$$= \frac{1}{N!} \det \begin{pmatrix} |n_1\rangle_1 & \dots & |n_N\rangle_1 \\ |n_1\rangle_N & \dots & |n_N\rangle_N \end{pmatrix} = |N_1, \dots, N_n \dots \rangle$$

number of fermions  
 in single particle state  
 ↓  
 \$|n\rangle\$  
 number of fermions in  
 single particle state \$|1\rangle\$  
 ↑

- The occupation numbers can only take the values  $N_i = 0, 1$ .
- For fixed  $N = \sum_i N_i$ , these particle number states span the  $N$ -particle Hilbert space  $\mathcal{H}_N^{\text{antisym}}$ , which consists only of antisymmetric states constructed from tensor products of single-particle states.
- For example, the space  $\mathcal{H}_2^{\text{antisym}}$  is spanned by  $|1,1,0,0,\dots\rangle, |1,0,1,0,\dots\rangle, |0,1,1,0,\dots\rangle$  etc.
- The direct sum  $\underbrace{\mathcal{H}_0^{\text{antisym}}}_{\text{identical to bosons}} \oplus \underbrace{\mathcal{H}_1^{\text{antisym}}}_{\text{}} \oplus \underbrace{\mathcal{H}_2^{\text{antisym}}}_{\text{}} \oplus \dots$  spans the Fock space  $\mathcal{F}^{\text{antisym}}$ .
- We proceed by studying the action of annihilation and creation operators on bosonic particle number states.
- Since all modes are independent, we have
 
$$a_n |N_1, N_2, \dots, N_n, \dots\rangle = \overline{N_n} |N_1, N_2, \dots, N_{n-1}, \dots\rangle$$

$$a_n^+ |N_1, N_2, \dots, N_n, \dots\rangle = \overline{N_{n+1}} |N_1, N_2, \dots, N_{n+1}, \dots\rangle,$$
 and the commutation relations are
 
$$[a_n, a_m] = \delta_{nm}, \quad [a_n, a_m^+] = [a_n^+, a_m^+] = 0.$$

- Furthermore, the particle number operator of the  $n$ -th mode obeys

$$\alpha_n^+ \alpha_n^- |N_1, N_2, \dots, N_n, \dots\rangle = N_n |N_1, N_2, \dots, N_n, \dots\rangle,$$

and a number state can be written as

$$|N_1, N_2, \dots, N_n, \dots\rangle = \frac{(\alpha_1^+)^{N_1}}{\Gamma(N_1!)} \frac{(\alpha_2^+)^{N_2}}{\Gamma(N_2!)} \frac{(\alpha_3^+)^{N_3}}{\Gamma(N_3!)} \dots |0\rangle.$$

↑  
vacuum

- The action of a creation operator on a symmetrised bosonic state  $|4^B\rangle$  with  $N$  particles is defined as follows:

$$\alpha_n^+ |4^B\rangle = \frac{1}{\Gamma(N+1)} \text{Sym} [|\bar{n}\rangle \otimes |4^B\rangle]$$

↑  
this means that the  
particle is inserted  
symmetrically into all  
 $N+1$  possible "positions"

↑  
creates boson  
in single-particle  
state  $|\bar{n}\rangle$

For example:

$$|4^B\rangle = \alpha_3^+ \alpha_4^+ |0\rangle = \frac{1}{\Gamma(2)} (|3\rangle_1 |4\rangle_2 + |4\rangle_1 |3\rangle_2) = |0,0,1,1, \dots\rangle$$

$$\begin{aligned} \hookrightarrow \alpha_3^+ |4^B\rangle &= \mathcal{N} \frac{1}{\Gamma(2)} (|3\rangle_1 |4\rangle_2 |3\rangle_3 + |4\rangle_1 |3\rangle_2 |3\rangle_3 + |3\rangle_1 |3\rangle_2 |4\rangle_3 + |4\rangle_1 |3\rangle_2 |3\rangle_3 \\ &\quad + |3\rangle_1 |3\rangle_2 |4\rangle_3 + |3\rangle_1 |4\rangle_2 |3\rangle_2) \\ &= \mathcal{N} \frac{1}{\Gamma(2)} (|3\rangle_1 |4\rangle_2 |3\rangle_3 + |3\rangle_1 |3\rangle_2 |4\rangle_3 + |4\rangle_1 |3\rangle_2 |3\rangle_3). \end{aligned}$$

↳ since  $a_3^+ |4^3\rangle = a_3^+ |0,0,1,1,\dots\rangle = \sqrt{2} |0,0,2,1,\dots\rangle$   
 it follows that  $\kappa = \frac{1}{\sqrt{3}}$ .

- The requirement that the application of a creation operator leads to symmetric state is "built into" the commutation relations.
- In order to treat a bosonic many-body system we therefore do not have to bother with the explicit construction of the many-particle states, but instead solely need to work with the algebraic properties of the creation and annihilation operators.
- Next, we turn to number states of fermionic systems and the action of fermionic annihilation and creation operators.
- Generalising the algebra of the latter to many modes leads to the anti-commutation relations

$$\{a_n, a_m^\dagger\} = \delta_{nm}, \quad \{a_n, a_m\} = \{a_n^\dagger, a_m^\dagger\} = 0$$

- A general number state is constructed

via

$$|N_1, N_2, \dots, N_n, \dots\rangle = \dots (a_n^+)^{N_n} \dots (a_2^+)^{N_2} (a_1^+)^{N_1} \underbrace{|0, 0, \dots, 0, \dots\rangle}_{= |0\rangle, \text{vacuum}}$$

- Since the occupation numbers  $N_i$  are either 0 or 1 there is no additional normalisation factor appearing.

- What is important to note is that we occupied in the construction of the above state the fermionic operators in a given order.

- This order is arbitrary, but it matters, since creation operators corresponding to different modes do not commute.

- In the following we therefore stick to the convention that the mode with the lowest index is filled first, and after that all other modes in ascending order.

- The action of a fermionic creation operator on an anti-symmetrised state  $|F\rangle$  with  $N$  particles is defined as

$$a_n^+ |14^F\rangle = \frac{1}{\sqrt{N+1}} \text{Antisym} [|n\rangle \otimes |14^F\rangle].$$

↑  
Creates fermion  
in mode  $|n\rangle$

↑  
single particle state is  
inserted such that the  
resulting wave function  
is anti-symmetric

For example:

$$\begin{aligned} |14^F\rangle &= a_4^+ a_3^+ |10\rangle = \underbrace{\frac{1}{\sqrt{2}} (|13\rangle_1 |14\rangle_2 - |14\rangle_1 |13\rangle_2)}_{= |10, 0, 1, 1, 0, \dots\rangle} = \frac{1}{\sqrt{2}} \det \begin{pmatrix} |13\rangle_1 & |13\rangle_2 \\ |14\rangle_1 & |14\rangle_2 \end{pmatrix} \\ &= -\frac{1}{\sqrt{2}} \det \begin{pmatrix} |14\rangle_1 & |14\rangle_2 \\ |13\rangle_1 & |13\rangle_2 \end{pmatrix} \quad \text{The order matters;} \\ &= -a_3^+ a_4^+ |10\rangle \quad (\neq -|10, 0, 1, 1, 0, \dots\rangle) \quad \text{we need to stick to our convention!} \end{aligned}$$

↳ the antisymmetrisation of the state  
is reflected in the anticommutator  
relations

- To add a particle in mode 5, one adds a row from below and a column  
from the right to the Slater determinant:

$$a_5^+ a_4^+ a_3^+ |10\rangle = \frac{1}{\sqrt{6}} \det - \begin{pmatrix} |13\rangle_1 & |13\rangle_2 & |13\rangle_3 \\ |14\rangle_1 & |14\rangle_2 & |14\rangle_3 \\ |15\rangle_1 & |15\rangle_2 & |15\rangle_3 \end{pmatrix}.$$

↑ normalisation factor changes:  $\frac{1}{\sqrt{2}} \frac{1}{\sqrt{2+1}}$

Using the properties of the Slater determinant one can then show that, e.g.

$$a_5^+ |0,0,1,1,0 \dots\rangle = a_5^+ a_4^+ a_3^+ |0\rangle = - a_4^+ a_5^+ a_3^+ |0\rangle.$$

Acting with a creation operator onto a general state thus yields

$$a_n^+ | \dots, \underset{n}{\overset{\uparrow}{0}}, \dots \rangle = (-1)^{n_n} | \dots, \underset{n}{\overset{\uparrow}{1}}, \dots \rangle,$$

with  $n_n = \sum_{m>n} N_m$  (number of fermions to the "left" of mode  $n$ ).

Likewise, one finds for the annihilation operator

$$a_n | \dots, \underset{n}{\overset{\uparrow}{1}}, \dots \rangle = (-1)^{n_n} | \dots, \underset{n}{\overset{\uparrow}{1}}, \dots \rangle,$$

such that the combination  $a_n^+ a_n$ , which

o. Lays

$$a_n^+ a_n | \dots, \underset{n}{\overset{\uparrow}{1}}, \dots \rangle = [(-1)^{n_n}]^2 | \dots, \underset{n}{\overset{\uparrow}{1}}, \dots \rangle = | \dots, \underset{n}{\overset{\uparrow}{1}}, \dots \rangle,$$

can be interpreted, like in the case of bosons, as number operator.

- To be able to work efficiently with the second quantisation formalism, we will now derive the representation of many-body operators in terms of creation and annihilation operators.

- We begin with operators which can be written as a sum of single-Body operators:

$$T = \sum_{\alpha=1}^N t_{\alpha} \xrightarrow{\text{Single-Body operator}} \text{acting on particle } \alpha$$

- The single-particle states  $|n\rangle_{\alpha}$  associated with the particle  $\alpha$  form a complete basis:

$$\mathbb{1} = \sum_n |n\rangle_{\alpha} \langle n|$$

- We can thus write

$$t_{\alpha} = \mathbb{1} t_{\alpha} \mathbb{1} = \sum_{mn} |m\rangle_{\alpha} \langle m| t_{\alpha} |n\rangle_{\alpha} \langle n|$$

- Note, that the matrix element

$$\langle m | t_{\alpha} | n \rangle_{\alpha} = \int d^3 \vec{r}_{\alpha} u_m^*(\vec{r}_{\alpha}) \stackrel{f}{\xrightarrow{\quad}} t(\vec{r}_{\alpha}) t_{\alpha} u_n(\vec{r}_{\alpha})$$

does not depend on  $\alpha$ , since it is the same for any particle.

$$\hookrightarrow \alpha \langle m | t_\alpha | n \rangle_\alpha = \langle m | t | n \rangle = t_{mn} .$$

- Therefore,  $t_\alpha = \sum_{mn} t_{mn} |m\rangle_\alpha \langle n|$

and

$$T = \sum_{mn} t_{mn} \sum_\alpha |m\rangle_\alpha \langle n| .$$

- In the following we show that

$$\sum_\alpha |m\rangle_\alpha \langle n| = a_m^+ a_n ,$$

i.e., we can express the sum over the outer product of single particle states as a product of an annihilation or creation operator, when applied to number states.

- Let's start with an example for bosons:

$$|2,0,1,0..\rangle = \frac{1}{\sqrt{3}} (|1\rangle_1 |1\rangle_2 |3\rangle_3 + |1\rangle_1 |3\rangle_2 |1\rangle_3 + |3\rangle_1 |1\rangle_2 |1\rangle_3 )$$

- Applying the operator  $\sum_\alpha |3\rangle_\alpha \langle 1|$  yields

$$(|3\rangle_1 \langle 1| + |3\rangle_2 \langle 1| + |3\rangle_3 \langle 1|) |2,0,1,0..\rangle$$

$$= (|3\rangle_1 \langle 1| + |3\rangle_2 \langle 1| + |3\rangle_3 \langle 1|) \frac{1}{\sqrt{3}} (|1\rangle_1 |1\rangle_2 |3\rangle_3 + |1\rangle_1 |3\rangle_2 |1\rangle_3 + |3\rangle_1 |1\rangle_2 |1\rangle_3 )$$

$$= \frac{1}{\sqrt{3}} (|3\rangle_1 |1\rangle_2 |3\rangle_3 + |3\rangle_1 |3\rangle_2 |1\rangle_3 + |1\rangle_1 |3\rangle_2 |3\rangle_3 + |3\rangle_1 |3\rangle_2 |1\rangle_3 + |1\rangle_1 |3\rangle_2 |3\rangle_3 + |3\rangle_1 |1\rangle_2 |3\rangle_3 )$$

$$= \frac{2}{\sqrt{3}} (|3\rangle_1 |1\rangle_2 |3\rangle_3 + |3\rangle_1 |3\rangle_2 |1\rangle_3 + |1\rangle_1 |3\rangle_2 |3\rangle_3 ) = 2 |1,0,2,0..\rangle$$

$$= a_3^+ a_1 |2,0,1,0..\rangle$$

For a general state

$$|N_1, \dots, N_n, \dots, N_m, \dots\rangle = \frac{1}{N! N_1! \dots N_n! \dots N_m!} \times$$

$$\times \sum_P \underbrace{|1\rangle_{P(1)} \dots |1\rangle_{P(N_1)}}_{N_1 \text{ terms}} \cdot \underbrace{|n\rangle_{P(1+n)} \dots |n\rangle_{P(\dots + N_n)}}_{N_n \text{ terms}} \cdot \underbrace{|m\rangle_{P(1+m)} \dots |m\rangle_{P(\dots + N_m)}}_{N_m \text{ terms}}$$

one finds

factor must be introduced  
to ensure correct normalisation

$$\left( \sum_\alpha \langle m | \alpha \right) |N_1, \dots, N_n, \dots, N_m \dots\rangle = N_m \frac{\overline{(N_m+1)! (N_m-1)!}}{\overline{N_m! N_{m-1}!}} |N_1, \dots, N_{m-1}, \dots, N_{m+1}, \dots\rangle$$

$$= \overline{N_{m+1}} \overline{N_m} |N_1, \dots, N_{m-1}, \dots, N_{m+1}, \dots\rangle$$

$$= a_m^+ a_n |N_1, \dots, N_n, \dots, N_m, \dots\rangle$$

This result also holds for fermions, so that we can write in general for a single-body operator:

$$T = \sum_{mn} t_{mn} a_m^+ a_n = \sum_{mn} \langle m | t | n \rangle a_m^+ a_n.$$

For example: Assume that  $T$  is a sum of single-body Hamiltonians,

$$T = H_0 = \sum_\alpha h_\alpha \quad \text{with } h |n\rangle = E_n |n\rangle.$$

$$\text{Then } H_0 = \sum_{mn} \underbrace{\langle m| h | n \rangle}_{E_n | n \rangle} a_m^+ a_n = \sum_n E_n a_n^+ a_n$$

$$= \sum_n E_n \hat{N}_n, \quad \begin{matrix} \leftarrow \text{number operator} \\ \hat{N}_n \end{matrix}$$

$$\text{and } H_0 |N_1, N_2, \dots\rangle = \left( \sum_n E_n N_n \right) |N_1, N_2, \dots\rangle$$

↑

The total energy is  
the sum over all  
occupation numbers  
multiplied by the  
energy of the corresponding  
single-particle state

- Let us now consider the representation of sums of two-body operators in the second quantisation formalism

- Such operators can be generally written

as

$$V = \frac{1}{2} \sum_{\substack{\alpha, \beta=1 \\ \alpha \neq \beta}}^N V_{\alpha \beta} \quad \begin{matrix} \leftarrow \text{operator acts on} \\ \text{two particles} \\ \text{simultaneously,} \\ \text{e.g. electron-electron} \\ \text{interaction} \end{matrix}$$

- We can now write, by inserting identities,

$$\begin{aligned}
 V &= \frac{1}{2} \sum_{\alpha, \beta} \sum_{m j n k} |m\rangle_\alpha \langle j|_\beta (\langle m | \langle j |) v_{\alpha \beta} (|n\rangle_\alpha \langle k|_\beta) \langle n | \langle k |
 \\ &= \frac{1}{2} \sum_{\alpha, \beta} \sum_{m j n k} |m\rangle_\alpha \langle j|_\beta \langle m | \langle n | v |n, k\rangle_\alpha \langle n | \beta \langle k |
 \\ &= \frac{1}{2} \sum_{m j n k} V_{m j n k} \sum_{\alpha, \beta} |m\rangle_\alpha \langle n | \langle j |_\beta \langle k |
 \end{aligned}$$

- We have used that the matrix element

$$V_{m j n k} = \langle m | j | v | n, k \rangle = \int d^3 r_\alpha \int d^3 r_\beta u_m^*(\vec{r}_\alpha) u_j^*(\vec{r}_\beta) v(\vec{r}_\alpha, \vec{r}_\beta) u_n(\vec{r}_\alpha) u_k(\vec{r}_\beta)$$

does not depend on  $\alpha$  and  $\beta$ .

- We now rewrite

$\nwarrow$  unconstrained summation

$$\sum_{\substack{\alpha, \beta \\ \alpha \neq \beta}} |m\rangle_\alpha \langle n | \langle j |_\beta \langle k | = \sum_{\alpha, \beta} |m\rangle_\alpha \langle n | \langle j |_\beta \langle k | - \underbrace{\sum_{\alpha} |m\rangle_\alpha \langle n | \langle j |_\alpha \langle k |}_{\delta_{nj}}$$

$$= a_m^+ a_n a_j^+ a_k - a_m^+ \delta_{nj} a_k$$

$$= a_m^+ a_n \delta_{nj}^+ a_k - \begin{cases} a_m^+ [a_n, a_j^+] a_k & \text{bosons} \\ a_m^+ \{a_n, a_j^+\} a_k & \text{fermions} \end{cases}$$

using  $\rightarrow$  =  $\begin{cases} a_m^+ a_j^+ a_n a_k & \text{bosons} \\ -a_m^+ a_j^+ a_n a_k & \text{fermions} \end{cases}$   
 (anti)commutators

- This yields the final result

$$V = \frac{1}{2} \sum_{mjk} V_{mjk} a_j^+ a_m^+ a_k,$$

and a typical Hamiltonian, which contains single and two-body terms reads in its second quantised form

$$H = \sum_{mn} \langle m|t|n\rangle a_m^+ a_n + \frac{1}{2} \sum_{mjk} \langle m,j|v|n,k\rangle a_j^+ a_m^+ a_k.$$

- We are now going to address the question concerning how the second quantised form of operators behaves under a change of basis.

- The new (old) basis shall be denoted as  $|l_n\rangle$   $|l\rangle$ , and we can expand the new basis states in terms of the old one according to

$$|l\rangle = \sum_n \underbrace{\langle n|l\rangle}_{\text{expansion coefficients}} |l_n\rangle$$

- Using the expansion coefficients, we can also relate the creation and annihilation operators of the old states ( $a_i, a_i^+$ ) with the new ones ( $b_\lambda, b_\lambda^+$ ).

$$b_\lambda^+ = \sum_n \langle n|\lambda\rangle a_n^+$$

$$b_\lambda = \sum_n \langle \lambda|n\rangle a_n \quad \xrightarrow{\text{adjoint equation}}$$

- The (anti)commutation relations remain unchanged when changing the basis, e.g. for bosons:

$$[b_\lambda, b_{\lambda'}^+] = \sum_{nm} \langle \lambda | n \rangle \langle m | \lambda' \rangle [a_n, a_m^+] \underbrace{\delta_{nm}}$$

$$= \sum_n \langle \lambda | n \rangle \langle n | \lambda' \rangle = \langle \lambda | \lambda' \rangle = \delta_{\lambda \lambda'}.$$

- The operator  $b_\lambda^+$  creates a single particle in the state  $|\lambda\rangle$ , and a general particle number state reads

$$|N_{\lambda_1}, \dots, N_{\lambda_i}, \dots\rangle = \frac{\dots (b_{\lambda_1}^+)^{N_{\lambda_1}} \dots (b_{\lambda_i}^+)^{N_{\lambda_i}}}{\dots \Gamma(N_{\lambda_1})! \dots \Gamma(N_{\lambda_i})!} |0 \dots 0\rangle \quad \begin{matrix} \text{new} \\ \text{basis} \end{matrix}$$

$$|N_{n_1}, \dots, N_{n_i}, \dots\rangle = \frac{\dots (a_{n_1}^+)^{N_{n_1}} \dots (a_{n_i}^+)^{N_{n_i}}}{\dots \Gamma(N_{n_1})! \dots \Gamma(N_{n_i})!} |0 \dots 0\rangle \quad \begin{matrix} \text{old} \\ \text{basis} \end{matrix}$$

vacuum state is  
the same in  
both bases

- The total number operator has the same appearance in both bases

$$\sum_\lambda b_\lambda^+ b_\lambda = \sum_{mn} \sum_\lambda \langle m|\lambda\rangle \langle \lambda|n\rangle a_m^+ a_n = \sum_{mn} \langle m|n\rangle a_m^+ a_n = \sum_n a_n^+ a_n = \hat{N}.$$

- Also, the form of a generic Hamiltonian remains unchanged:

$$H = \sum_{\lambda\lambda'} \langle \lambda | t | \lambda' \rangle b_\lambda^+ b_{\lambda'} + \frac{1}{2} \sum_{\lambda\lambda' \mu\mu'} \langle \lambda, \lambda' | v | \mu, \mu' \rangle b_\lambda^+ b_\lambda^+ b_\mu^- b_{\mu'}^-.$$

- A particular important basis is associated with the real-space representations:

$$b_{\vec{r}}^+ = \sum_n \underbrace{\langle n | \vec{r} \rangle}_{\text{↑}} a_n^+ = \underbrace{\sum_n u_n^*(\vec{r})}_{\text{↑}} a_n^+ \equiv \psi(\vec{r})$$

Spatial mode  
(wave function)

↑  
adjoint field operator

- The field operator obeys the commutation relations

$$\begin{aligned} [\psi(\vec{r}), \psi^+(\vec{r}')] &= \sum_{nn'} u_n(\vec{r}) u_{n'}^*(\vec{r}') [a_n, a_{n'}^+] \\ &= \underbrace{\sum_n u_n(\vec{r}) u_n^*(\vec{r})}_{\text{Completeness relation}} = \delta^3(\vec{r} - \vec{r}') \end{aligned}$$

and

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

- Fermions follow the corresponding anticommutation relations.

- A particle number state has now the form

$$|N_{\vec{r}_1}, \dots, N_{\vec{r}_i}, \dots\rangle = \frac{-(4^+(\vec{r}_1))^{\bar{N}_{\vec{r}_1}} \dots (4^+(\vec{r}_i))^{\bar{N}_{\vec{r}_i}} |0,0,\dots\rangle}{\dots \sqrt{N_{\vec{r}_1}!} \dots \sqrt{N_{\vec{r}_i}!}},$$

and the  $N_{\vec{r}_i}$  give the number of particles found at position  $\vec{r}_i$ .

- The particle number operator we can write by introducing the particle density operator

$$\rho(\vec{r}) = 4^+(\vec{r}) 4(\vec{r})$$

$$\begin{aligned} \hat{N} &= \int d^3 r \rho(\vec{r}) = \int d^3 \vec{r} \left( \sum_m u_m^*(\vec{r}) a_m^\dagger \right) \left( \sum_n u_n(\vec{r}) a_n \right) \\ &= \sum_{mn} a_m^\dagger a_n \underbrace{\int d^3 r u_m^*(\vec{r}) u_n(\vec{r})}_{\delta_{mn}} = \sum_n a_n^\dagger a_n. \end{aligned}$$

- For a single-particle one obtains the representation:

$$\begin{aligned} \sum_{mn} \langle m | t | n \rangle a_m^\dagger a_n &= \sum_{mn} a_m^\dagger a_n \int d^3 r u_m^*(\vec{r}) t u_n(\vec{r}) \\ &= \int d^3 r 4^+(\vec{r}) t 4(\vec{r}) \end{aligned}$$

↑ spatial representation  
of the operator  $t$

For example:

$$H_0 = \sum_{\alpha=1}^N \left( -\frac{\hbar^2}{2m} \Delta_\alpha + V_{ext}(\vec{r}_\alpha) \right)$$

$$= \int d^3\vec{r} \Psi^+(\vec{r}) \left( -\frac{\hbar^2}{2m} \Delta + V_{ext}(\vec{r}) \right) \Psi(\vec{r})$$

looks like the expectation value for a single particle energy, but the wave functions are replaced by field operators

For a two-particle operator one obtains the representation:

$$\begin{aligned} V &= \frac{1}{2} \sum_{m,j,n,k} \langle m,j | v | n,k \rangle a_j^+ a_m^+ a_n a_k \\ &= \frac{1}{2} \sum_{m,j,n,k} a_j^+ a_m^+ \int d^3\vec{r}_0 \int d^3\vec{r}'_1 u_m^*(\vec{r}_0) u_j^*(\vec{r}') v(\vec{r}_1, \vec{r}') u_n(\vec{r}_0) u_k(\vec{r}') a_n a_k \\ &= \frac{1}{2} \underbrace{\int d^3\vec{r} \int d^3\vec{r}'_1 \Psi^+(\vec{r}) \Psi^+(\vec{r}')}_{(\Psi(\vec{r}), \Psi(\vec{r}'))^+} v(\vec{r}, \vec{r}') \Psi(\vec{r}) \Psi(\vec{r}') \end{aligned}$$

- Rather often it is useful to introduce creation and annihilation operators in momentum space.
- Considering a finite quantisation volume  $V=L \times L \times L$ , the eigenvalues of the momentum operator are

$$\vec{p} = \frac{2\pi\hbar}{L} \begin{pmatrix} k_x \\ k_y \\ k_z \end{pmatrix}.$$

The corresponding eigenstates are plane waves

$$\langle \vec{r} | \vec{p} \rangle = \frac{1}{\sqrt{V}} e^{i \frac{\vec{p} \cdot \vec{r}}{\hbar}}.$$

The expansion of momentum eigenstates in terms of spatial eigenfunctions is

$$|\vec{p}\rangle = \int d^3r \langle \vec{r} | \vec{p} \rangle |\vec{r}\rangle$$

and thus

$$a_{\vec{p}}^+ = \frac{1}{\sqrt{V}} \int d^3r e^{i \frac{\vec{p} \cdot \vec{r}}{\hbar}} \psi^+(\vec{r})$$

$$a_{\vec{p}}^- = \frac{1}{\sqrt{V}} \int d^3r e^{-i \frac{\vec{p} \cdot \vec{r}}{\hbar}} \psi(\vec{r})$$

$\underbrace{\quad}_{\text{Creation and annihilation operators of a particle with momentum } \vec{p}}$

$\underbrace{\quad}_{\text{field operators}}$

The inverse transformation is

$$\psi^+(\vec{r}) = \frac{1}{\sqrt{V}} \sum_{\vec{p}} e^{-i \frac{\vec{p} \cdot \vec{r}}{\hbar}} a_{\vec{p}}^+, \quad \psi(\vec{r}) = \frac{1}{\sqrt{V}} \sum_{\vec{p}} e^{i \frac{\vec{p} \cdot \vec{r}}{\hbar}} a_{\vec{p}}^-,$$

from which follows

$$\begin{aligned} [a_{\vec{p}}, a_{\vec{p}'}^+] &= \frac{1}{V} \int d^3r \int d^3r' e^{-i \frac{\vec{p} \cdot \vec{r}}{\hbar}} e^{i \frac{\vec{p}' \cdot \vec{r}'}{\hbar}} [\psi(\vec{r}), \psi^+(\vec{r}')] \\ &= \frac{1}{V} \int d^3r e^{i \frac{\vec{p} \cdot \vec{r}}{\hbar} (\vec{r}' - \vec{p}')} = \frac{1}{V} V \delta_{\vec{p}, \vec{p}'} = \delta_{\vec{p}, \vec{p}'} \end{aligned}$$

For fermions, again, the appropriate anticommutator holds.

Examples:

- Kinetic energy:

$$\begin{aligned} \int d^3\vec{r} \psi^+(\vec{r}) \left(-\frac{\hbar^2}{2\mu} \Delta\right) \psi(\vec{r}) &= \frac{1}{V} \sum_{\vec{p}\vec{p}'} a_{\vec{p}}^+ a_{\vec{p}'} \int d^3\vec{r} e^{-i\frac{\vec{p}\cdot\vec{r}}{\hbar}} \left(-\frac{\hbar^2}{2\mu} \Delta\right) e^{i\frac{\vec{p}'\cdot\vec{r}}{\hbar}} \\ &= \frac{1}{V} \sum_{\vec{p}\vec{p}'} \frac{\hbar^2}{2\mu} a_{\vec{p}}^+ a_{\vec{p}'} \underbrace{\int d^3\vec{r} e^{-i(\vec{p}-\vec{p}')\cdot\frac{\vec{r}}{\hbar}}}_{V \delta_{\vec{p}\vec{p}'}} \\ &= \sum_{\vec{p}} \frac{\hbar^2}{2\mu} a_{\vec{p}}^+ a_{\vec{p}} \end{aligned}$$

- Single particle potential,

$$\int d^3\vec{r} \psi^+(\vec{r}) V_{ext}(\vec{r}) \psi(\vec{r}) = \frac{1}{V} \sum_{\vec{p}\vec{p}'} \tilde{V}_{ext}(\vec{p}-\vec{p}') a_{\vec{p}}^+ a_{\vec{p}'}$$

with  $\tilde{V}_{ext}(\vec{q}) = \int d^3\vec{r} V_{ext}(\vec{r}) e^{-i\frac{\vec{q}\cdot\vec{r}}{\hbar}}$

being the Fourier transformed potential

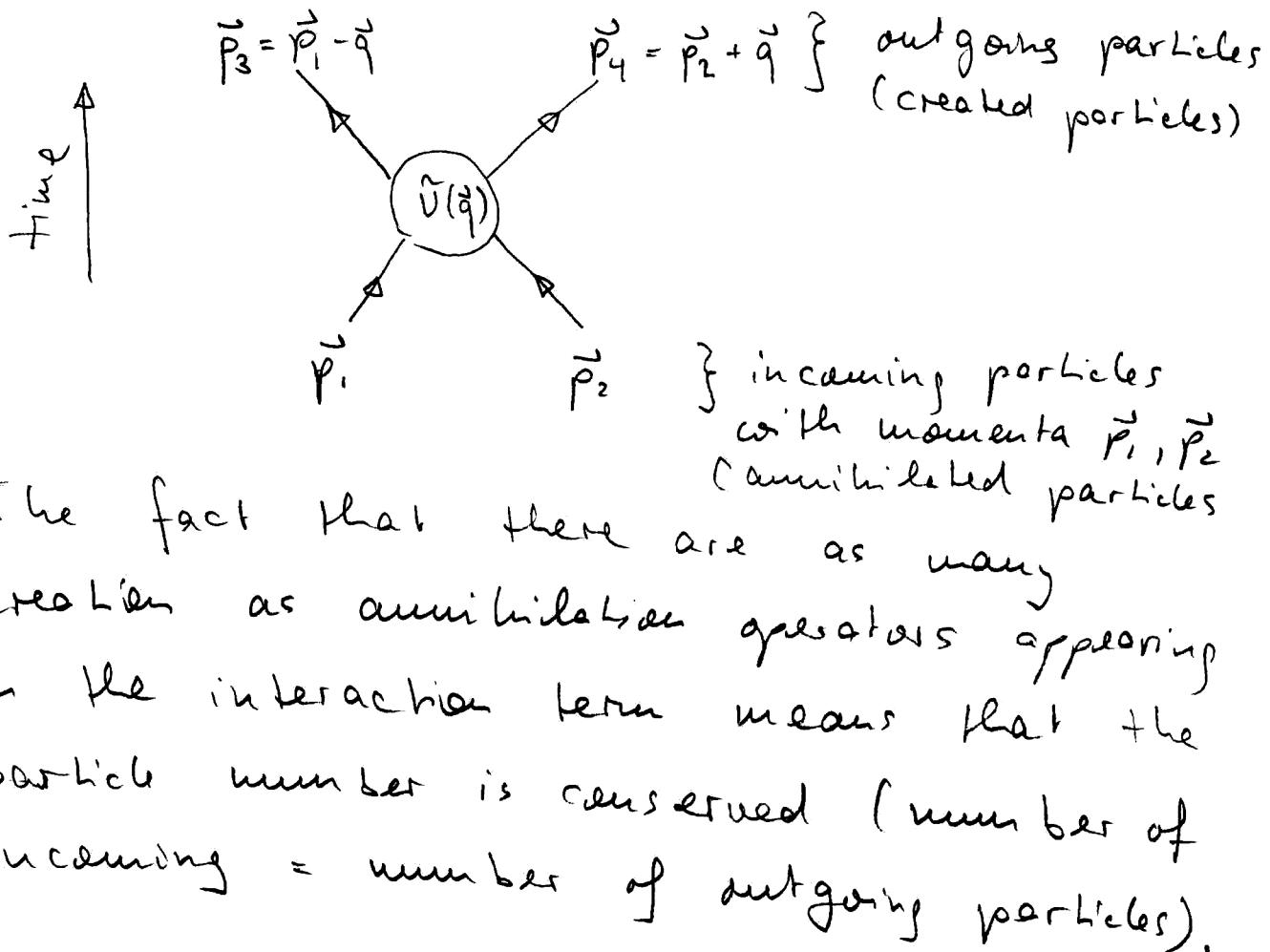
- Two-particle interaction,  $v(\vec{r}, \vec{r}') = v(\vec{r}-\vec{r}')$

$$\frac{1}{2} \int d^3\vec{r} \int d^3\vec{r}' \psi^+(\vec{r}') \psi^+(\vec{r}) v(\vec{r}-\vec{r}') \psi(\vec{r}) \psi(\vec{r}') = \frac{1}{2V} \sum_{\vec{p}_1 \vec{p}_2 \vec{q}} \tilde{v}(\vec{q}) a_{\vec{p}_1+\vec{q}}^+ a_{\vec{p}_2+\vec{q}}^+ a_{\vec{p}_1} a_{\vec{p}_2}$$

with  $\tilde{v}(\vec{q}) = \int d^3\vec{r} v(\vec{r}) e^{-i\frac{\vec{q}\cdot\vec{r}}{\hbar}}$

- The second quantisation formalism in momentum space is of great importance in scattering theory.

- The Fourier transform of the interaction potential for a given momentum  $\vec{q}$  determines for example the strength of a scattering event of the type



- The fact that there are as many creation as annihilation operators appearing in the interaction term means that the particle number is conserved (number of incoming = number of outgoing particles).
- We will now revisit the Harbree-Fock approach using the second quantisation formalism.
- The Hamiltonian of a many-electron atom is

$$H = \sum_{\alpha=1}^{N=7} \left( -\frac{\hbar^2}{2\mu} \Delta_\alpha - \frac{Ze^2}{4\pi\epsilon_0 |\vec{r}_\alpha|} \right) + \frac{1}{2} \sum_{\alpha \neq \beta=1}^{N=7} \frac{e^2}{4\pi\epsilon_0 |\vec{r}_\alpha - \vec{r}_\beta|}$$

$t_\alpha$                            $V_{\alpha\beta}$

- The trial state for the electrons is a (anti-symmetrized) particle number state, i.e.

$$|4\rangle = a_1^+ \dots a_n^+ |0, \dots 0\rangle.$$

- The expectation value of the energy for this state is

$$\langle H \rangle = \sum_{mn} \langle mltl n \rangle \langle 4 | a_m^+ a_n | 4 \rangle + \frac{1}{2} \sum_{m j n k} \langle m j l V l n, k \rangle \langle 4 | a_j^+ a_m^+ a_n a_k | 4 \rangle.$$

- For the matrix elements we obtain

$$\langle 4 | a_m^+ a_n | 4 \rangle = \delta_{mn} \quad (a_m^+ a_n | 4 \rangle \text{ is orthogonal to } | 4 \rangle \text{ unless } m=n)$$

$$\langle 4 | a_j^+ a_m^+ a_n a_k | 4 \rangle = \underbrace{\delta_{mn}}_{\substack{\text{indices of one annihilation and} \\ \text{creation operators must be the same}}} \delta_{jk} \langle 4 | a_k^+ a_m^+ a_n a_k | 4 \rangle$$

$$+ \delta_{mk} \delta_{jn} \langle 4 | a_n^+ a_j^+ a_n a_k | 4 \rangle$$

$$= (-\delta_{mn} \delta_{jk} + \delta_{mk} \delta_{jn}) \langle 4 | \underbrace{a_n^+ a_k^+ a_n a_k}_{= -a_n a_k^+ + \delta_{nk}} | 4 \rangle$$

$$= (\delta_{mn} \delta_{jk} - \delta_{mk} \delta_{jn}) \langle 4 | \underbrace{a_n^+ a_n}_{N_n} \underbrace{a_k^+ a_k}_{N_k} | 4 \rangle$$

$$= \delta_{mn} \delta_{jk} - \delta_{mk} \delta_{jn}$$

$\uparrow$   
does not contribute,  
since all indices will  
be the same

- We thus find

$$\sum_{mn} \langle m|t|n\rangle \langle 4|\alpha_m^+ \alpha_n|4\rangle = \sum_n \langle n|t|n\rangle = \sum_n t_{nn}$$

and

$$\begin{aligned} \frac{1}{2} \sum_{mjk} \langle m_j|v|n_k\rangle \langle 4|\alpha_j^+ \alpha_m^+ \alpha_n \alpha_k|4\rangle &= \frac{1}{2} \sum_{\substack{m,k=1 \\ m \neq k}} (\langle m_k|v|m_k\rangle - \langle m_k|v|k_m\rangle) \\ &= \frac{1}{2} \sum_{\substack{m,k=1 \\ m \neq k}} (v_{mk} - v_{km}) . \end{aligned}$$

• Translating this to the real space representation yields the result that we previously obtained:

$$\begin{aligned} \langle 4|H|4\rangle &= \sum_{n=1}^{N=2} \int d^3r u_n^*(\vec{r}) \left[ -\frac{\hbar^2}{2\mu} \Delta - \frac{ze^2}{4\pi\epsilon_0 |\vec{r}|} \right] u_n(\vec{r}) \\ &+ \frac{1}{2} \sum_{\substack{m,k=1 \\ m \neq k}} \int d^3r \int d^3r' \frac{e^2}{4\pi\epsilon_0 |\vec{r}-\vec{r}'|} \underbrace{\left( |u_m(\vec{r})|^2 |u_k(\vec{r}')|^2 - \int_{S_{m,k}} u_m^*(\vec{r}) u_k^*(\vec{r}') u_k(\vec{r}) u_m(\vec{r}') \right)}_{\text{we made explicit here, that the interaction is diagonal in the spin}} \end{aligned}$$

- As another application of the second quantisation formalism, we consider the Fermi gas.
- A system of  $N$  non-interacting fermions are fixed in a box of volume  $V = L \times L \times L$  is described by the Hamiltonian
- $$H_{kin} = \sum_{\vec{p}, s} \frac{\hbar^2}{2\mu} \alpha_{\vec{p}s}^+ \alpha_{\vec{p}s} , \quad \vec{p} = \frac{2\pi\hbar}{L} \begin{pmatrix} k_x \\ k_y \\ k_z \end{pmatrix}$$
- ↑ spin projection
- momentum quantum numbers ↓

- The smaller the momentum, the smaller the energy.
- Therefore, the ground state is constructed by filling up all momentum states, starting from  $\vec{p} = 0$  and ending at  $|\vec{p}| = p_F$ , where  $p_F$  is the Fermi momentum, which depends on  $N$  and  $V$ .
- Ground state:  $| \phi_0 \rangle = \prod_{\vec{p}} \prod_{s} a_{\vec{p},s}^+ | 0 \rangle$

- The total particle number obeys

$$N = \sum_{\vec{p},s} N_{\vec{p},s} = \sum_{\vec{p},s} \langle \phi_0 | \hat{N}_{\vec{p},s} | \phi_0 \rangle = \sum_{\substack{\vec{p},s \\ |\vec{p}| \leq p_F}} 1 = \sum_{\substack{\vec{p} \\ |\vec{p}| \leq p_F}} 2$$

$$= \frac{2V}{(2\pi\hbar)^3} \underbrace{\int_{|\vec{p}| \leq p_F} d^3 p}_\text{volume of a sphere with radius } p_F = \frac{V}{3\pi^2\hbar^3} p_F^3$$

volume of a sphere with radius  $p_F$

↳ Fermi momentum:  $p_F^3 = \frac{3\pi^2\hbar^3}{V} \frac{N}{V} = 3\pi^2\hbar^3 \frac{N}{V}$

- The total energy is given by
- $$E = \sum_{\substack{\vec{p},s \\ |\vec{p}| \leq p_F}} \frac{\vec{p}^2}{2\mu} = \frac{2V}{(2\pi\hbar)^3} \int_{|\vec{p}| \leq p_F} d^3 p \frac{\vec{p}^2}{2\mu} = \frac{2V}{(2\pi\hbar)^3} \frac{4\pi}{2\mu} \int_0^{p_F} dp p^4 = \frac{V}{10\pi^2\hbar^3} p_F^5$$
- ↑  
particle density
- $$= \frac{3}{5} N \frac{p_F^2}{2\mu} = \frac{3}{5} N E_F$$
- ↑ Fermi energy

- (133)

  - We now turn to the more interesting case of an interacting Fermi gas, which is embedded in a uniform positive charge density  $\rho = e \frac{N}{V}$ , which mimics ions of a metal.
  - This charge density is chosen such that it cancels the charge of the electrons, so that overall the system is neutral.
  - This is the so-called Jellium model.
  - Its Hamiltonian is

$$H = H_{\text{kin}} + H_{e,\text{iden}} + H_{ee} + E_{\text{ion,ion}}$$

↑  
 kinetic energy  
 of electrons      ↑  
 electron  
 ion interaction      ↑  
 electron-  
 electron  
 interaction      ↑  
 ion-ion  
 interaction  
 (energy shift)

- We assume the the ground state  $| \phi_0 \rangle$  of a non interacting Fermi gas is a good approximation for this system and calculate the contribution of the perturbations  $H_{\text{spin}}$  and  $H_{\text{ex}}$  in first order perturbation theory.

• Electron-ion interaction:

$$\langle \phi_0 | H_{\text{e,ion}} | \phi_0 \rangle = \langle \phi_0 | \frac{1}{V} \sum_{\vec{p}\vec{p}'} \sum_{ss'} \tilde{V}_{\text{ext}}(\vec{p}-\vec{p}') a_{\vec{p}s}^+ a_{\vec{p}'s'}^- | \phi_0 \rangle,$$

with  $\tilde{V}_{\text{ext}}(\vec{q}) = \int d^3r V_{\text{ext}}(\vec{r}) e^{i\vec{q} \cdot \vec{r}}$  and

$$V_{\text{ext}}(\vec{r}) = -e \int d^3r' \frac{e(\vec{r}')}{{4\pi\epsilon_0} |\vec{r}-\vec{r}'|} = -\sqrt{\int d^3r' \frac{e^2}{{4\pi\epsilon_0} |\vec{r}-\vec{r}'|}}.$$

This yields:

$$\begin{aligned} \langle \phi_0 | H_{\text{e,ion}} | \phi_0 \rangle &= \frac{1}{V} \sum_{\vec{p}\vec{p}'} \sum_{ss'} \tilde{V}_{\text{ext}}(\vec{p}-\vec{p}') \underbrace{\langle \phi_0 | a_{\vec{p}s}^+ a_{\vec{p}'s'}^- | \phi_0 \rangle}_{\delta_{\vec{p}\vec{p}'} \delta_{ss'} N_{\vec{p},s}} \\ &= 1 \text{ for } |\vec{p}| \leq p_F \\ &= \frac{1}{V} \sum_{\substack{\vec{p}s \\ |\vec{p}| \leq p_F}} \tilde{V}_{\text{ext}}(0) = \frac{N}{V} \int d^3r V_{\text{ext}}(\vec{r}) \\ &= -\sqrt{2} \underbrace{\int d^3r \int d^3r' \frac{e^2}{{4\pi\epsilon_0} |\vec{r}-\vec{r}'|}}_{\text{large constant}} \\ &= -\sqrt{2} \end{aligned}$$

• Electron-electron interaction:

$$\langle \phi_0 | H_{\text{ee}} | \phi_0 \rangle = \frac{1}{2} \int d^3r \int d^3r' \underbrace{v(|\vec{r}-\vec{r}'|)}_{\text{pair correlation function}} \sum_{ss'} \underbrace{\langle \phi_0 | 4_{s1}^+(\vec{r}) 4_s^+(\vec{r}) 4_s^-(\vec{r}) 4_{s1}^-(\vec{r}') | \phi_0 \rangle}_{\text{pair correlation function}}$$

$$G_{ss'}(\vec{r}-\vec{r}') = \left(\frac{V}{2}\right)^2 \begin{cases} 1 & , s \neq s' \\ 1 - \left(\frac{3(\sin x - x \cos x)}{x^3}\right)^2 , & s = s' \end{cases}$$

with  $x = \frac{p_F}{k} |\vec{r}-\vec{r}'|$

With the Coulomb potential

$$v(|\vec{r} - \vec{r}'|) = \frac{e^2}{4\pi\epsilon_0 |\vec{r} - \vec{r}'|} \quad \text{this yields}$$

$$\langle \phi_0 | H_{\text{ee}} | \phi_0 \rangle = \frac{1}{2} \int d^3 r \int d^3 r' v(|\vec{r} - \vec{r}'|) \left[ 2 \left( \frac{v}{2} \right)^2 + 2 \left( \frac{v}{2} \right)^2 \left( 1 - \left( \frac{3(\sin x - x \cos x)}{x^3} \right)^2 \right) \right]$$

$$= \frac{v^2}{2} U - \frac{9v^2}{4} \frac{e^2 p_F}{4\pi\epsilon_0 t} \int d^3 r \int d^3 r' \frac{(8\sin x - x \cos x)^2}{x^7}$$

$$= \frac{v^2}{2} U - \frac{9}{4} v^2 V \frac{e^2 p_F}{4\pi\epsilon_0 t} \frac{\pi t^3}{p_F^3}$$

$$= \frac{v^2}{2} U - \frac{3}{4\pi} \frac{e^2}{4\pi\epsilon_0 t} p_F N$$

Ion-ion interaction energy shift:

$$\begin{aligned} E_{\text{ion-ion}} &= \frac{1}{2} \int d^3 r \int d^3 r' \frac{p(r) p(r')}{4\pi\epsilon_0 |\vec{r} - \vec{r}'|} \\ &= \frac{v^2}{2} \int d^3 r \int d^3 r' \frac{e^2}{4\pi\epsilon_0 |\vec{r} - \vec{r}'|} = \frac{v^2}{2} U, \end{aligned}$$

cancels all other  $U$ -dependent terms

Adding all contributions together, yields

$$E_{\text{ground}} = \langle \phi_0 | H | \phi_0 \rangle = \frac{3}{5} E_F N - v^2 U + \frac{v^2}{2} U - \frac{3}{4\pi} \frac{e^2}{4\pi\epsilon_0 t} p_F N + \frac{v^2}{2} U.$$

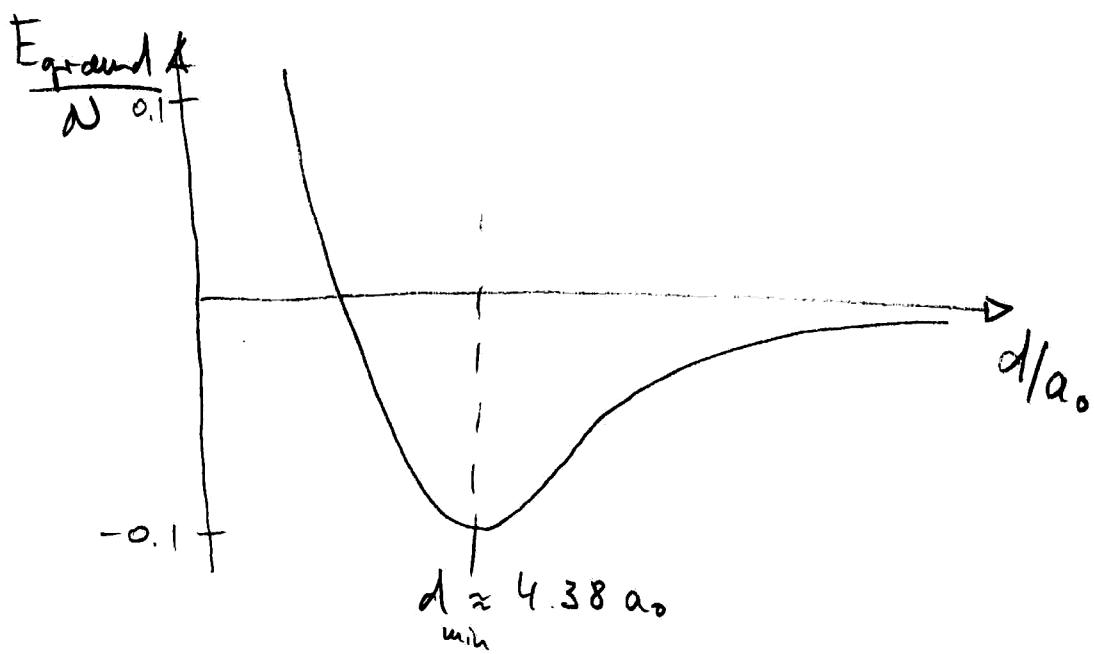
$$\begin{aligned} \hookrightarrow \frac{E_{\text{ground}}}{N} &= \frac{3}{5} E_F - \frac{3}{4\pi} \frac{e^2}{4\pi\epsilon_0 t} p_F \\ &= E_{Ryd} \left[ \frac{3}{5} \left( \frac{9\pi}{4} \right)^{2/3} \left( \frac{a_0}{d} \right)^2 - \frac{3}{2\pi} \left( \frac{9\pi}{4} \right)^{1/3} \left( \frac{a_0}{d} \right) \right] \end{aligned}$$

Bohr's radius

Pydberg energy

with  $d = \sqrt[3]{\frac{9\pi}{4} \frac{t}{p_F}}$ .

- The quantity  $d$  is a length, which (136) characterises the typical distance between electrons.
- It depends on  $p_F$  and therefore on  $N$  and  $V$ .
- Interestingly, the function  $\frac{E_{\text{ground}}}{N}$  has a minimum and one would therefore expect that an electron gas adjusts  $p_F$  ( $N$  and  $V$ ) such that the ground state energy is minimised.



- The minimisation yields  $d_{\min} \approx 4.38 a_0$  and  $\frac{E_{\text{ground}}}{N} \Big|_{d=d_{\min}} \approx -0.1 \text{ Ryd}$ .
- This is comparable with actual metals, such as sodium ( $d = 3.96 a_0$ ) and potassium ( $d = 4.86 a_0$ ).