Thus, the results (3.47) and (3.48) can be combined to the operator identity

$$\boxed{\hat{\Pi}_{ij} = \sum_{\alpha=1}^{N} |i\rangle_\alpha \langle j|_\alpha = \hat{a}_i^\dagger \hat{a}_j} \tag{3.49}$$

which, together with the definition (3.46), proves the theorem[14].

For the special case that the orbitals are eigenfunctions of an operator, $\hat{b}_\alpha|\phi_i\rangle = b_i|\phi_i\rangle$—such as the single-particle hamiltonian, the corresponding matrix is diagonal, $b_{ij} = b_i\delta_{ij}$, and the representation (3.43) simplifies to

$$\hat{B}_1 = \sum_{i=1}^{\infty} b_i\, \hat{a}_i^\dagger \hat{a}_i = \sum_{i=1}^{\infty} b_i\, \hat{n}_i, \tag{3.50}$$

where b_i are the eigenvalues of $\hat{b}$. Equation (3.50) naturally generalizes the familiar spectral representation of quantum mechanical operators to the case of many-body systems with arbitrary variable particle number.

Two-particle operators

A two-particle operator is of the form

$$\hat{B}_2 = \frac{1}{2!} \sum_{\alpha\neq\beta=1}^{N} \hat{b}_{\alpha,\beta}, \tag{3.51}$$

where $\hat{b}_{\alpha,\beta}$ acts only on particles α and β. An example is the operator of the pair interaction, $\hat{b}_{\alpha,\beta} \to w(|\mathbf{r}_\alpha - \mathbf{r}_\beta|)$. We introduce again matrix elements, now with respect to two-particle states composed as products of single-particle orbitals, which belong to the two-particle Hilbert space $\mathcal{H}_2 = \mathcal{H}_1 \otimes \mathcal{H}_1$,

$$b_{ijkl} = \langle ij|\hat{b}|kl\rangle, \tag{3.52}$$

Theorem: The second quantization representation of a two-particle operator is given by

$$\boxed{\hat{B}_2 = \frac{1}{2!} \sum_{i,j,k,l=1}^{\infty} b_{ijkl}\, \hat{a}_i^\dagger \hat{a}_j^\dagger \hat{a}_l \hat{a}_k} \tag{3.53}$$

Proof:
We expand $\hat{b}$ for an arbitrary pair α, β into a basis of two-particle orbitals

[14] See problem 2.

$|ij\rangle = |\phi_i\rangle|\phi_j\rangle$,

$$\hat{b} = \sum_{i,j,k,l=1}^{\infty} |ij\rangle\langle ij|\hat{b}|kl\rangle\langle kl| = \sum_{i,j,k,l=1}^{\infty} |ij\rangle\langle kl|\, b_{ijkl},$$

leading to the following result for the total two-particle operator,

$$\hat{B}_2 = \frac{1}{2!}\sum_{i,j,k,l=1}^{\infty} b_{ijkl} \sum_{\alpha\neq\beta=1}^{N} |i\rangle_\alpha |j\rangle_\beta \langle k|_\alpha \langle l|_\beta. \tag{3.54}$$

The second sum is readily transformed, using the property (3.49) of the sigle-particle states. We first extend the summation over the particles to include $\alpha = \beta$,

$$\begin{aligned}
\sum_{\alpha\neq\beta=1}^{N} |i\rangle_\alpha |j\rangle_\beta \langle k|_\alpha \langle l|_\beta &= \sum_{\alpha=1}^{N} |i\rangle_\alpha \langle k|_\alpha \sum_{\beta=1}^{N} |j\rangle_\beta \langle l|_\beta - \delta_{k,j} \sum_{\alpha=1}^{N} |i\rangle_\alpha \langle l|_\alpha \\
&= \hat{a}_i^\dagger \hat{a}_k \hat{a}_j^\dagger \hat{a}_l - \delta_{k,j}\, \hat{a}_i^\dagger \hat{a}_l \\
&= \hat{a}_i^\dagger \left\{ \hat{a}_j^\dagger \hat{a}_k + \delta_{k,j} \right\} \hat{a}_l - \delta_{k,j}\, \hat{a}_i^\dagger \hat{a}_l \\
&= \hat{a}_i^\dagger \hat{a}_j^\dagger \hat{a}_k \hat{a}_l.
\end{aligned}$$

In the third line we have used the commutation relation (3.36). After exchanging the order of the two annihilators (they commute) and inserting this expression into Eq. (3.54), we obtain the final result (3.53)[15].

General many-particle operators

The above results are directly extended to more general operators involving K particles out of N

$$\boxed{\hat{B}_K = \frac{1}{K!} \sum_{\alpha_1 \neq \alpha_2 \neq \ldots \alpha_K = 1}^{N} \hat{b}_{\alpha_1,\ldots\alpha_K},} \tag{3.55}$$

and which have the second quantization representation

$$\boxed{\hat{B}_K = \frac{1}{K!} \sum_{j_1\ldots j_k m_1 \ldots m_k = 1}^{\infty} b_{j_1\ldots j_k m_1 \ldots m_k}\, \hat{a}_{j_1}^\dagger \ldots \hat{a}_{j_k}^\dagger \hat{a}_{m_k} \ldots . \hat{a}_{m_1}} \tag{3.56}$$

[15]Note that the order of the creation operators and of the annihilators, respectively, is arbitrary. In Eq. (3.53) we have chosen an ascending order of the creators (same order as the indices of the matrix element) and a descending order of the annihilators, since this leads to an expression which is the same for Bose and Fermi statistics, cf. Sec. 3.4.1.

where we used the general matrix elements with respect to k-particle product states, $b_{j_1 \dots j_k m_1 \dots m_k} = \langle j_1 \dots j_k | \hat{b} | m_1 \dots m_k \rangle$. Note again the inverse ordering of the annihilation operators. Obviously, the result (3.56) includes the previous examples of single and two-particle operators as special cases.

Comment: of course, our goal is to compute expectation values of operators that correctly incorporate the spin statistics of the particles. It may look, therefore, counter-intuitive, that the second quantization representation of $\hat{B}_K, K \geq 2$ includes matrix elements with non-(anti-)symmetric K-particle states (product states). However, this is not a contradiction. The spin statistics are taken care of by the creation and annihilation operates. The matrix elements can be computed with any set of states, as long as they span the relevant K-particle Hilbert space[16].

3.4 Second quantization for fermions

We now turn to particles with half-integer spin, i.e. fermions, which are described by anti-symmetric wave functions and obey the Pauli principle, cf. Sec. 3.2.3.

3.4.1 Creation and annihilation operators for fermions

As for bosons we wish to introduce creation and annihilation operators that should again allow for the construction of any many-body state out of the vacuum state, according to [cf. Eq. (3.37)]

$$|n_1, n_2, \dots \rangle = \Lambda^-_{1\dots N} |i_1 \dots i_N\rangle = \left(\hat{a}_1^\dagger\right)^{n_1} \left(\hat{a}_2^\dagger\right)^{n_2} \dots |0\rangle. \qquad n_i = 0, 1, \quad (3.57)$$

Due to the Pauli principle we expect that there will be no additional prefactors resulting from multiple occupations of orbitals, as in the case of bosons[17]. So far we do not know how these operators look like explicitly. Their definition has to make sure that the N-particle states have the correct anti-symmetry and that application of any creator (or annihilator) more than once will return zero.

Example: $N = 2$. To solve this problem, consider two fermions which can occupy the orbitals k or l. The two-particle state has the symmetry $|kl\rangle = -|lk\rangle$, upon particle exchange. The anti-symmetrized state is constructed of

[16]This is the same approach as has been used in the construction of the N-particle wave function of an interacting system in Sec. 3.2.5.

[17]The prefactors are always equal to unity because $1! = 1$.

the product state of particle 1 in state k and particle 2 in state l and has the properties

$$\Lambda^{-}_{1\ldots N}|kl\rangle = \hat{a}^{\dagger}_{l}\hat{a}^{\dagger}_{k}|0\rangle = |11\rangle = -\Lambda^{-}_{1\ldots N}|lk\rangle = -\hat{a}^{\dagger}_{k}\hat{a}^{\dagger}_{l}|0\rangle, \tag{3.58}$$

i.e., it changes sign upon exchange of the particles (third equality). This indicates that the state depends on the order in which the orbitals are filled, i.e., on the order of action of the two creation operators. One possible choice is used in the above equation and immediately implies that[18]

$$\hat{a}^{\dagger}_{k}\hat{a}^{\dagger}_{l} + \hat{a}^{\dagger}_{l}\hat{a}^{\dagger}_{k} = [\hat{a}^{\dagger}_{k}, \hat{a}^{\dagger}_{l}]_{+} = 0, \qquad \forall k, l, \tag{3.59}$$

where we have introduced the *anti-commutator*[19]. In the special case, $k = l$, we immediately obtain $\left(\hat{a}^{\dagger}_{k}\right)^2 = 0$, for an arbitrary state, in agreement with the Pauli principle. Calculating the hermitean adjoint of Eq. (3.59) we obtain that the anti-commutator of two annihilators vanishes as well,

$$[\hat{a}_{k}, \hat{a}_{l}]_{+} = 0, \qquad \forall k, l. \tag{3.60}$$

We expect that this property holds for any two orbitals k, l and for any N-particle state that involves these orbitals since our consideration did not depend on a specific case.

Now we can introduce an explicit definition of the fermionic creation operator which has all these properties. The operator creating a fermion in orbital k of a general many-body state is defined as[20]

$$\boxed{\hat{a}^{\dagger}_{k}|\ldots, n_k, \ldots\rangle = (1 - n_k)(-1)^{\alpha_k}|\ldots, n_k + 1, \ldots\rangle, \quad \alpha_k = \sum_{l<k} n_l} \tag{3.61}$$

where the prefactor explicitly enforces the Pauli principle, and the sign factor takes into account the position of the orbital k in the many-fermion state and the number of fermions standing "to the left" of the "newly created" particle, cf. Fig. 3.6. In other words, with α_k pair exchanges (anti-commutations) the particle would move from the leftmost place to the position (e.g. according to an ordering with respect to the orbital energies E_k) of orbital k in the N-particle state. We now derive the annihilation operator by inserting a complete

[18]We can leave out the state $|0\rangle$ on which the operators act because our derivation can be repeated for any state.

[19]This was introduced by P. Jordan and E. Wigner in 1927. Sometimes the anticommutator is denoted with curly brackets, $\{\hat{A}, \hat{B}\}$.

[20]There can be other conventions which differ from ours by the choice of the exponent α_k which, however, is irrelevant for physical observables.

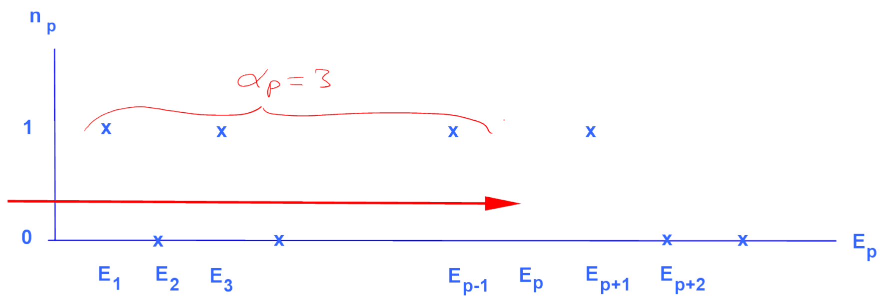

Abbildung 3.6: Illustration of the phase factor α in the fermionic creation and annihilation operators. A fermion is added to orbital "p" (red arrow) and has to be moved past three singly occupied orbitals ($n_p = 1$) with lower energy. This requires $\alpha_p = 3$ pair exchanges, i.e. a sign change will occur. Particles in orbitals with higher energy do not influence the sign. The single-particle orbitals are assumed to be in a definite order (e.g. with respect to the energy eigenvalues).

set of anti-symmetric states and using (3.61)

$$\begin{aligned}
\hat{a}_k|\ldots,n_k,\ldots\rangle &= \sum_{\{n'\}} |\{n'\}\rangle\langle\{n'\}|\hat{a}_k|\ldots,n_k,\ldots\rangle = \\
&= \sum_{\{n'\}} |\{n'\}\rangle\langle\{n\}|\hat{a}_k^\dagger|\{n'\}\rangle^* \\
&= \sum_{\{n'\}} (1-n'_k)(-1)^{\alpha'_k}\delta^k_{\{n'\},\{n\}}\delta_{n_k,n'_k+1}|\{n'\}\rangle \\
&= (2-n_k)(-1)^{\alpha_k}|\ldots,n_k-1,\ldots\rangle \\
&\equiv n_k(-1)^{\alpha_k}|\ldots,n_k-1,\ldots\rangle
\end{aligned}$$

where, in the third line, we used definition (3.33). Also, $\alpha'_k = \alpha_k$ because the sum involves only occupation numbers that are not altered. Note that the factor $2 - n_k = 1$, for $n_k = 1$. However, for $n_k = 0$ the present result is not correct, as it should return zero. To this end, in the last line we have added the factor n_k that takes care of this case. At the same time this factor does not alter the result for $n_k = 1$. Thus, the factor $2 - n_k$ can be skipped entirely, and we obtain the expression for the fermionic annihilation operator of a particle in orbital k

$$\boxed{\hat{a}_k|\ldots,n_k,\ldots\rangle = n_k(-1)^{\alpha_k}|\ldots,n_k-1,\ldots\rangle} \tag{3.62}$$

Using the definitions (3.61) and (3.62) one readily proves the anti-commutation relations given by the

Theorem: The creation and annihilation operators defined by Eqs. (3.61) and (3.62) obey the relations

$$[\hat{a}_i,\hat{a}_k]_+ = [\hat{a}_i^\dagger,\hat{a}_k^\dagger]_+ = 0, \qquad \forall i,k, \tag{3.63}$$

$$\left[\hat{a}_i,\hat{a}_k^\dagger\right]_+ = \delta_{i,k}. \tag{3.64}$$

Proof of relation (3.63):

Consider, the case of two annihilators and the action on an arbitrary anti-symmetric state

$$[\hat{a}_i,\hat{a}_k]_+|\{n\}\rangle = (\hat{a}_i\hat{a}_k + \hat{a}_k\hat{a}_i)\,|\{n\}\rangle, \tag{3.65}$$

and consider first case $i=k$. Inserting the definition (3.62), we obtain

$$(\hat{a}_k)^2\,|\{n\}\rangle \sim n_k\hat{a}_k|n_1\ldots n_k-1\ldots\rangle = 0,$$

and thus the anti-commutator vanishes as well. Consider now the case[21] $i<k$:

$$\begin{aligned}\hat{a}_i\hat{a}_k|\{n\}\rangle &= \hat{a}_i n_k(-1)^{\sum_{l<k}n_l}|n_1\ldots n_k-1\ldots\rangle = \\ &= n_i n_k(-1)^{\sum_{l<k}n_l}(-1)^{\sum_{l<i}n_l}|n_1\ldots n_i-1\ldots n_k-1\ldots\rangle.\end{aligned}$$

Now we compute the result of the action of the exchanged operator pair

$$\begin{aligned}\hat{a}_k\hat{a}_i|\{n\}\rangle &= \hat{a}_k n_i(-1)^{\sum_{l<i}n_l}|n_1\ldots n_i-1\ldots\rangle = \\ &= n_i n_k(-1)^{\sum_{l<i}n_l}(-1)^{\sum_{l<k}n_l-1}|n_1\ldots n_i-1\ldots n_k-1\ldots\rangle,\end{aligned}$$

The only difference compared to the first result is in the additional -1 in the second exponent. It arises because, upon action of $\hat{a}_k$ after $\hat{a}_i$, the number of particles to the left of k is already reduced by one. Thus, the two expressions differ just by a minus sign, which proves vanishing of the anti-commutator.

The proof of relation (3.64) proceeds analogously and is subject of Problem 3, cf. Sec. 3.9.

Thus we have proved all anti-commutation relations for the fermionic operators and confirmed that the definitions (3.61) and (3.62) obey all properties required for fermionic field operators. We can now proceed to use these operators to bring arbitrary quantum-mechanical operators into second quantized form in terms of fermionic orbitals.

[21]This covers the general case of $i \neq k$, since i and k are arbitrary.

Particle number operators

As in the case of bosons, the operator

$$\boxed{\hat{n}_i = \hat{a}_i^\dagger \hat{a}_i} \tag{3.66}$$

is the *occupation number operator* for orbital i because, for $n_i = 0, 1$,

$$\hat{a}_i^\dagger \hat{a}_i |\{n\}\rangle = \hat{a}_i^\dagger (-1)^{\alpha_i} n_i |n_1 \dots n_i - 1 \dots\rangle = n_i[1 - (n_i - 1)]|\{n\}\rangle,$$

where the prefactor equals n_i, for $n_i = 1$ and zero otherwise. Thus, the anti-symmetric state $|\{n\}\rangle$ is an eigenstate of $\hat{n}_i$ with the eigenvalue coinciding with the occupation number n_i of this state[22].
The *total particle number operator* is defined as

$$\hat{N} = \sum_{i=1}^{\infty} \hat{n}_i = \sum_{i=1}^{\infty} \hat{a}_i^\dagger \hat{a}_i, \tag{3.67}$$

because its action yields the total particle number:
$\hat{N}|\{n\}\rangle = \sum_{i=1}^{\infty} n_i |\{n\}\rangle = N|\{n\}\rangle$.

Single-particle operators

Consider now again a single-particle operator

$$\hat{B}_1 = \sum_{\alpha=1}^{N} \hat{b}_\alpha, \tag{3.68}$$

and let us find its second quantization representation.
Theorem: The second quantization representation of a single-particle operator is given by

$$\boxed{\hat{B}_1 = \sum_{i,j=1}^{\infty} b_{ij}\, \hat{a}_i^\dagger \hat{a}_j} \tag{3.69}$$

Proof:
As for bosons, cf. Eq. (3.44), we have

$$\hat{B}_1 = \sum_{\alpha=1}^{N} \sum_{i,j=1}^{\infty} b_{ij} |i\rangle_\alpha \langle j|_\alpha = \sum_{i,j=1}^{\infty} b_{ij} \hat{\Pi}_{ij}, \tag{3.70}$$

[22]This result, together with the anti-commutation relations for the operators a and $a^\dagger$ proves the consistency of the definitions (3.61) and (3.62).

where $\hat{\Pi}_{ij}$ was defined by (3.42), and it remains to show that $\hat{\Pi}_{ij} = \hat{a}_i^\dagger \hat{a}_j$, for fermions as well. To this end we consider action of $\hat{\Pi}_{ij}$ on an anti-symmetric state, taking into accont that $\hat{\Pi}_{ij}$ commutes with the anti-symmetrization operator $\Lambda^-_{1\dots N}$, Eq. (3.14),

$$\hat{\Pi}_{ij}|\{n\}\rangle = \frac{1}{\sqrt{N!}} \sum_{\alpha=1}^{N} \sum_{\pi \epsilon S_N} \mathrm{sign}(\pi) |i\rangle_\alpha \langle j|_\alpha \cdot |j_1\rangle_{\pi(1)} |j_2\rangle_{\pi(2)} \dots |j_N\rangle_{\pi(N)}. \quad (3.71)$$

If the product state does not contain the orbital $|j\rangle$ expression (3.71) vanishes, due to the orthogonality of the orbitals. Otherwise, let $j_k = j$. Then $\langle j|j_k\rangle = 1$, and the orbital $|j_k\rangle$ will be replaced by $|i\rangle$, unless the state $|i\rangle$ is already present, then we again obtain zero due to the Pauli principle, i.e.

$$\hat{\Pi}_{ij}|\{n\}\rangle \quad \sim \quad (1 - n_i) n_j \left| \{n\}^i_j \right\rangle, \quad (3.72)$$

where we used the notation (3.46). What remains is to figure out the sign change due to the removal of a particle from the i-th orbital and creation of one in the k-th orbital. To this end we first "move" the (empty) orbital $|j\rangle$ past all orbitals to the left occupied by $\alpha_j = \sum_{p<j} n_p$ particles, requiring just α_j pair permutations and sign changes. Next we move the "new" particle to orbital "i" past $\alpha_i = \sum_{p<i} n_p$ particles occupying the orbitals with an energy lower then E_i leading to α_i pair exchanges and sign changes[23]. Taking into account the definitions (3.61) and (3.62) we obtain[24]

$$\boxed{\hat{\Pi}_{ij}|\{n\}\rangle = (-1)^{\alpha_i + \alpha_j} (1 - n_i) n_j \left| \{n\}^i_j \right\rangle = \hat{a}_i^\dagger \hat{a}_j |\{n\}\rangle} \quad (3.73)$$

which, together with the equation (3.70), proves the theorem. Thus, the second quantization representation of single-particle operators is the same for bosons and fermions.

Two-particle operators

As for bosons, we now derive the second quantization representation of a two-particle operator $\hat{B}_2$.

[23]Note that, if $i > j$, the occupation numbers occuring in α_i have changed by one compared to those in α_j.

[24]One readily verifies that this result applies also to the case $j = i$. Then the prefactor is just $[1 - (n_j - 1)]n_j = n_j$, and $\alpha_i = \alpha_j$, resulting in a plus sign

$$\hat{\Pi}_{jj}|\{n\}\rangle \quad = \quad n_j \; |\{n\}\rangle = \hat{a}_j^\dagger \hat{a}_j |\{n\}\rangle.$$

Theorem: The second quantization representation of a two-particle operator is given by

$$\boxed{\hat{B}_2 = \frac{1}{2!}\sum_{i,j,k,l=1}^{\infty} b_{ijkl}\, \hat{a}_i^\dagger \hat{a}_j^\dagger \hat{a}_l \hat{a}_k} \tag{3.74}$$

Proof:
As for bosons, we expand $\hat{B}$ into a basis of two-particle orbitals $|ij\rangle = |\phi_i\rangle|\phi_j\rangle$,

$$\hat{B}_2 = \frac{1}{2!}\sum_{i,j,k,l=1}^{\infty} b_{ijkl} \sum_{\alpha\neq\beta=1}^{N} |i\rangle_\alpha |j\rangle_\beta \langle k|_\alpha \langle l|_\beta, \tag{3.75}$$

and transform the second sum

$$\begin{aligned}
\sum_{\alpha\neq\beta=1}^{N} |i\rangle_\alpha |j\rangle_\beta \langle k|_\alpha \langle l|_\beta &= \sum_{\alpha=1}^{N} |i\rangle_\alpha \langle k|_\alpha \sum_{\beta=1}^{N} |j\rangle_\beta \langle l|_\beta - \delta_{k,j} \sum_{\alpha=1}^{N} |i\rangle_\alpha \langle l|_\alpha \\
&= \hat{a}_i^\dagger \hat{a}_k \hat{a}_j^\dagger \hat{a}_l - \delta_{k,j}\, \hat{a}_i^\dagger \hat{a}_l \\
&= \hat{a}_i^\dagger \left\{ -\hat{a}_j^\dagger \hat{a}_k + \delta_{k,j} \right\} \hat{a}_l - \delta_{k,j}\, \hat{a}_i^\dagger \hat{a}_l \\
&= -\hat{a}_i^\dagger \hat{a}_j^\dagger \hat{a}_k \hat{a}_l.
\end{aligned}$$

In the third line we have used the anti-commutation relation (3.64). After exchanging the order of the two annihilators, which now leads to a sign change and, inserting this expression into Eq. (3.75), we obtain the final result (3.74).

Comment: from the derivation it is clear that there exist a variety of equivalent representations of two-particle operators that are obtained by interchanging pairs of field operators. Here we note one that is obtained when we retain the original alternating order of creation and annihilation operators. Introducing the single-particle density operator $\hat{n}_{ij} = \hat{a}_i^\dagger \hat{a}_j$

$$\hat{B}_2 = \frac{1}{2!}\sum_{i,j,k,l=1}^{\infty} b_{ijkl} \left\{ \hat{n}_{ik}\hat{n}_{jl} - \delta_{kj}\hat{n}_{il} \right\}. \tag{3.76}$$

General many-particle operators

The above results are directly extended to a general K-particle operator, $K \leq N$, which was defined in Eq. (3.55). Its second quantization representation is found to be

$$\boxed{\hat{B}_K = \frac{1}{K!}\sum_{j_1\dots j_k m_1\dots m_k=1}^{\infty} b_{j_1\dots j_k m_1\dots m_k}\, \hat{a}_{j_1}^\dagger \dots \hat{a}_{j_k}^\dagger \hat{a}_{m_k} \dots .\hat{a}_{m_1}} \tag{3.77}$$