The second quantization method for indistinguishable particles

Valery Shchesnovich

Lecture Notes for postgraduates

UFABC, 2010
“All I saw hast kept safe in a written record, here thy worth and eminent endowments come to proof.”

Dante Alighieri, Inferno
Contents

1 Creation and annihilation operators for the system of indistinguishable particles 4
  1.1 The permutation group and the states of a system of indistinguishable particles 5
  1.2 Dimension of the Hilbert space of a system of indistinguishable particles 8
  1.3 Definition and properties of the creation and annihilation operators 9
  1.4 The Fock space 13
  1.5 The representations of state vectors and operators 16
    1.5.1 N-particle wave-functions 16
    1.5.2 The second-quantization representation of operators 18
    1.5.3 Examples 21
  1.6 Evolution of operators in the Heisenberg picture 22
  1.7 Statistical operators of indistinguishable particles 24
    1.7.1 The averages of the s-particle operators 27
    1.7.2 The general structure of the one-particle statistical operator 29

2 Quadratic Hamiltonian and the diagonalization 31
  2.1 Diagonalization of the Hamiltonian quadratic in the fermion operators 32
  2.2 Diagonalization of the Hamiltonian quadratic in the boson operators 36
    2.2.1 Diagonalization of the quadratic bosonic Hamiltonian possessing a zero mode 41
  2.3 Long range order, condensation and the Bogoliubov spectrum of weakly interacting Bose gas 44
    2.3.1 The excitation spectrum of weakly interacting Bose gas in a box 47
    2.3.2 The excitation spectrum of an interacting Bose gas in an external potential 50
  2.4 The Jordan-Wigner transformation: fermionization of interacting 1D spin chains 54
Chapter 1

Creation and annihilation operators for the system of indistinguishable particles

The properties of the permutation group are reviewed. The projectors on the symmetric and anti-symmetric subspaces of the Hilbert space of the system of identical particles are considered. The dimension of the physical Hilbert space of a system of indistinguishable identical particles is calculated. The creation and annihilation operators are introduced starting from the states they create or annihilate. The properties of the creation and annihilation operators are derived from their definition. The basis of the physical Hilbert space is expressed using the creation operators applied to the vacuum state. The representation of the arbitrary vectors in the physical Hilbert space is given in terms of these basis states. It is shown how to expand the s-particle observables in the operator basis composed of the creation and annihilation operators, which corresponds to the “bra-ket” vector basis of the observables describing distinguishable particles. The evolution equation for the creation and annihilation operators is derived. The statistical operators are also introduced and related to the average of the observables. Some examples are provided.
1.1 The permutation group and the states of a system of indistinguishable particles

We will say that the particles are identical if they have the same properties. On the other hand, the particles are considered indistinguishable if they cannot be labelled with an index.

The Hilbert space of a system consisting of \( N \) identical (distinguishable!) particles is constructed from the tensor product of the states describing each particle alone, for instance if \( N \) particles are found in the states labelled as \( X_\alpha, X_\beta, \ldots, X_\gamma \) we have

\[
| X_\alpha^{(1)}, X_\beta^{(2)}, \ldots, X_\gamma^{(N)} \rangle \equiv | X_\alpha \rangle | X_\beta \rangle \cdots | X_\gamma \rangle.
\] (1.1)

Here and below we will use the upper index for labelling of the particles, while in the tensor product (the r.h.s. of Eq. (1.1)) the position of the vector identifies to which particle it corresponds. The arbitrary vector of the Hilbert space of \( N \) identical particles is then given by an arbitrary linear combination of the vectors defined in Eq. (1.1).

A permutation \( P \) of \( N \) ordered elements \( (X_1, X_2, \ldots, X_N) \) is an operation which changes the order of the elements. A good way to visualize it is to think that the elements are placed in the string of boxes labelled by the natural numbers and the operation \( P \) swaps the contents of the boxes. For instance, we can write

\[
(X_1, X_2, \ldots, X_N) \xrightarrow{P} (X_{i_1}, X_{i_2}, \ldots, X_{i_N}),
\] (1.2)

i.e. implying that \( i_k \rightarrow k \) or \( P(i_k) = k \). In other words, under the action of \( P \) of Eq. (1.2) the content from the \( i_k \)-th box goes to the box labelled with the index \( k \) (while the content of the \( k \)-th box goes somewhere else). The permutation operations form a group, since the composition of two permutations is also a permutation and each permutation has the inverse one. The trivial permutation, which leaves the order unchanged, will be defined by \( I \). The simplest permutation operation is the transposition, i.e. the interchange of just two elements from the ordered set, for example for \( i \neq j \) we define \( P_{ij}(i) = j \) and \( P_{ij}(j) = i \) with the rest of the boxes preserving their content under \( P_{ij} \). This permutation will be denoted below as simply \( (i, j) \). Note that it is inverse to itself \( (i, j)(i, j) = I \). The following useful property

\[
(i, j) = (i, 1)(j, 2)(1, 2)(i, 1)(j, 2)
\] (1.3)

can be verified by simple calculation. Moreover, it is easy to see that an arbitrary permutation can be represented as composition of the transpositions (moreover, any permutation can be written as a composition of the elementary transpositions of the form \( (i, i + 1) \)). Finally, there are \( N! \) of all permutations of a set of \( N \) elements.

The signature of a permutation, denoted as \( \varepsilon(P) \), is defined as a mapping of the permutation group to the group of two elements \( \{-1, 1\} \), where the usual product is the group operation on the latter set. Using Eq. (1.3) and the group
property one can establish that there are just two possible ways to attribute a signature to the permutation: the trivial one, i.e. $P \rightarrow 1$ and the one which attributes the signature $-1$ to the permutation $(1,2)$ and, by Eq. (1.3), to any permutation being a transposition, $\varepsilon(P_{ij}) = -1$ for $i \neq j$ (in this case, the signature is called the parity). To verify that it is indeed possible to define the parity of $P$ (as preserving the group operation mapping to the set \{-1,1\}) one can produce its explicit expression, given as a product of the partial signatures, i.e.

$$\varepsilon(P) \equiv \prod_{i<j} \text{sgn}[P(j) - P(i)],$$

(1.4)

where \text{sgn} is the sign function and the permutation $P$ acts on the ordered set $(1,2,\ldots,N)$, e.g. as in Eq. (1.2). First, to verify the group property consider the composition of two permutations $P_2$ and $P_1$, i.e. the permutation $P_3(k) = P_2(P_1(k))$ or $P_3 = P_2 \circ P_1$. We have

$$\varepsilon(P_2 \circ P_1) = \prod_{i<j} \text{sgn}[P_2(P_1(j)) - P_2(P_1(i))]
= \prod_{i<j} \text{sgn}[P_1(j) - P_1(i)] \prod_{P_1(i)<P_1(j)} \text{sgn}[P_2(P_1(j)) - P_2(P_1(i))]
= \varepsilon(P_1)\varepsilon(P_2).$$

Second, obviously $\varepsilon(P_{12}) = -1$. It is clear that the parity $\varepsilon(P) = (-1)^s$, where $s$ is the number of the transpositions in a representation of $P$ (as a byproduct, we get that any two such representations must have the same parity of the number of transpositions).

Let us now consider the permutation operation as acting on the Hilbert space of $N$ identical particles. Since it is a linear space, the permutation operation $P$ now becomes a linear operator (for which we will use the same notation $P$). Namely, we define the action of the operator $P$ corresponding to the permutation in Eq. (1.2) as follows

$$P \mid X_1 \rangle \mid X_2 \rangle \cdots \mid X_N \rangle \equiv \mid X_{i_1} \rangle \mid X_{i_2} \rangle \cdots \mid X_{i_N} \rangle,$$

(1.5)

or in the product form

$$P \mid X_1 \rangle \mid X_2 \rangle \cdots \mid X_N \rangle = \mid X_{i_1} \rangle \mid X_{i_2} \rangle \cdots \mid X_{i_N} \rangle.$$

It is clear from this definition that the permutation operator is unitary, i.e. $P^\dagger = P^{-1}$.

If the particles are considered as indistinguishable, the interchange of any two must not affect the state of the system (except for a constant phase). Thus if $\mid S \rangle$ is the state of such a system, we must have $P \mid S \rangle = e^{i\varphi(P)} \mid S \rangle$, where the phase depends on the permutation $P$. On the other hand, for any transposition $P_{ij} = (1,2)$ we must have $P_{ij}^2 \mid S \rangle = \mid S \rangle$, since $P_{ij}^2 = I$. Thus $\varphi(P_{ij}) = 0$ or $\pi$ and, due to Eq. (1.3), it is the same phase for any transposition. In other words,
one should use the state which are either symmetric or anti-symmetric in the interchange of two particles. The particles which are described by the symmetric states are called \textit{bosons} and the ones described by the anti-symmetric states are called \textit{fermions}. The states which satisfy the property $P | S \rangle = \varepsilon(P) | S \rangle$, i.e. symmetric and anti-symmetric states, will be called the physical states of the indistinguishable particles, or simply the physical states.

To construct a physical state from a product state of $N$ identical particles one can use the projector operators $S_N$ and $A_N$ defined as follows

$$S_N \equiv \frac{1}{N!} \sum_P P, \quad A_N \equiv \frac{1}{N!} \sum_P \varepsilon(P)P,$$

(1.6)

where the summation runs over all transpositions of the set of $N$ elements (note that in the sum we have operators, while in the index of the summation the corresponding transpositions). The projector property is readily verified:

$$S_N^2 = \left( \frac{1}{N!} \right)^2 \sum_P P \sum_{P'} P' = \left( \frac{1}{N!} \right)^2 \sum_P \sum_{P\circ P'} PP'$$

$$= \frac{1}{N!} \sum_{P\circ P'} PP' = S_N$$

and

$$A_N^2 = \left( \frac{1}{N!} \right)^2 \sum_P \varepsilon(P)P \sum_{P'} \varepsilon(P')P' = \left( \frac{1}{N!} \right)^2 \sum_P \sum_{P\circ P'} \varepsilon(P)\varepsilon(P')PP'$$

$$= \frac{1}{N!} \sum_{P\circ P'} \varepsilon(PP')PP' = A_N.$$

Moreover, the two projectors in Eq. (1.6) are orthogonal, i.e. the symmetric and anti-symmetric subspaces are orthogonal (which is a necessary property if they are to describe two different types of particles, bosons and fermions). Indeed, by similar calculation one gets

$$S_N A_N = \left( \frac{1}{N!} \right)^2 \sum_P P \sum_{P'} \varepsilon(P')P' = \left( \frac{1}{N!} \right)^2 \sum_P \varepsilon(P) \sum_{P\circ P'} \varepsilon(P)\varepsilon(P')PP'$$

$$= \left( \frac{1}{N!} \sum_P \varepsilon(P) \right) A_N = 0,$$

since one can divide all the permutation operators into two classes by multiplication by $P_{12}$: $\hat{P} = P_{12}P$, where the operators related by $P_{12}$ have the signatures of different sign.

The projectors $S_N$ and $A_N$ are also Hermitian, which is a consequence of the unitarity of the permutation operators, $P^\dagger = P^{-1}$ and the property $\varepsilon(P) = \varepsilon(P^{-1})$. 

7
\( \varepsilon(P^{-1}) \). It is easy to see that only in the case of just two particles the sum of these projectors is the identity operator, i.e. \( S_2 + A_2 = I_2 \).

To unify the consideration, we will use the same notation \( \varepsilon(P) \) for the signature in the boson and fermion cases. Thus we will write the “generalized symmetrization” as

\[
S_N^\varepsilon = \frac{1}{N!} \sum_P \varepsilon(P) P,
\]

where \( \varepsilon(P) = 1 \) for the case of \( S_N \).

The states of \( N \) indistinguishable particles can be given as linear combinations of the following states

\[
| X_1, X_2, \ldots, X_N \rangle = S_N^\varepsilon \{ | X_1^{(1)} , X_2^{(2)} , \ldots , X_N^{(N)} \rangle \}
= S_N^\varepsilon \{ | X_1 \rangle | X_2 \rangle \ldots | X_N \rangle \},
\]

where (and below) we use the notation \( | X_1, X_2, \ldots, X_N \rangle \) for a symmetric or anti-symmetric state of \( N \) particles occupying the single-particle states labelled by \( X_1, X_2, \ldots, X_N \) (not necessarily different). Explicitly, we have (compare with Eq. (1.2))

\[
| X_1, X_2, \ldots, X_N \rangle = \frac{1}{N!} \sum_P \varepsilon(P) | X_{P^{-1}(1)} \rangle | X_{P^{-1}(2)} \rangle \ldots | X_{P^{-1}(N)} \rangle
\]  

(1.9)

Note that this vector is not normalized, in general. If two single-particle states are identical, \( X_i = X_j \) then the corresponding anti-symmetric state is absent (one obtains zero on the r.h.s. of Eq. (1.9)) – this is nothing but the Pauli exclusion principle for fermions.

### 1.2 Dimension of the Hilbert space of a system of indistinguishable particles

In the previous section we have considered the states of a system of \( N \) indistinguishable particles. Consider now the Hilbert space of such states, the physical Hilbert space for below. It is a subspace of the product of \( N \) identical single-particle Hilbert spaces, \( H \otimes H \otimes H \otimes \ldots \otimes H \). We will denote the Hilbert space of \( N \) indistinguishable particles as \( H_N \equiv S_N^\varepsilon \{ H \otimes H \otimes H \otimes \ldots \otimes H \} \). Assuming that the dimension of \( H \) be \( d \), i.e. \( \dim(H) = d \), let us find the dimension of the Hilbert space \( H_N \). The dimension of the Hilbert space \( H_N^{(B)} \) for bosons, occupying \( d \) single-particle states is the total amount of various distributions of the \( N \) indistinguishable particles between the \( d \) states, such that there are exactly \( m_j \) particles in the \( j \)-th state, i.e. (using the usual \( \delta \)-symbol)

\[
\dim(H_N^{(B)}) = \sum_{m_1=0}^{N} \ldots \sum_{m_d=0}^{N} \delta_{\sum_{j=1}^{d} m_j , N} = \sum_{m_1=0}^{N} \ldots \sum_{m_d=0}^{N} \left( \frac{2\pi}{2\pi} \right) e^{i \theta (\sum_{j=1}^{d} m_j - N)}
\]

\[= \frac{2\pi}{2\pi} \int_0^{2\pi} e^{i \theta (\sum_{j=1}^{d} m_j - N)} d\theta \]
\[ N \sum_{m=0}^{N} \ldots \sum_{n=0}^{N} \int_{0}^{2\pi} \frac{d\theta}{2\pi} e^{-iN\theta} \prod_{j=1}^{d} e^{i m_j \theta} = \int_{0}^{2\pi} \frac{d\theta}{2\pi} e^{-iN\theta} \left( \sum_{m=0}^{N} e^{i m \theta} \right)^{\!d} = \int_{0}^{2\pi} \frac{d\theta}{2\pi} e^{-iN\theta} \left( \frac{1-e^{i(N+1)\theta}}{1-e^{i\theta}} \right)^{\!d} \].

Now we change the variable to \( z = e^{i\theta} \) and use the theorem of residues to calculate the integral (there is a pole at \( z = 0 \), while at \( z = 1 \) the integrand is regular)

\[ \dim(\mathcal{H}^{(B)}_{N}) = \frac{1}{2\pi} \int_{|z|=1} dz \, z^{-N-1} \left( \frac{1-z^{N+1}}{1-z} \right)^{\!d} = \frac{1}{N!} \frac{d^{N}}{dz^{N}} \left( \frac{1-z^{N+1}}{1-z} \right) \bigg|_{z=0} = \frac{1}{N!} [d(d+1) \ldots (d+N-1)]. \]

Therefore, for bosons we have obtained

\[ \dim(\mathcal{H}^{(B)}_{N}) = \frac{1}{N!} [d(d+1) \ldots (d+N-1)] = C^{\!N}_{N+d-1}, \quad (1.10) \]

where the symbol \( C^{\!m}_{n} \) is defined as \( C^{\!m}_{n} = \frac{m!}{(m-n)!n!} \).

On the other hand, in the case of fermions by applying the Pauli exclusion principle (and the indistinguishability of the particles), we get

\[ \dim(\mathcal{H}^{(F)}_{N}) = \begin{cases} 0, & N > d \\ \frac{1}{N!} [d(d-1) \ldots (d-N+1)], & N \leq d \end{cases} = C^{\!N}_{d}. \quad (1.11) \]

### 1.3 Definition and properties of the creation and annihilation operators

The creation \( a^{+}_{\beta} \) and annihilation \( a^{-}_{\beta} \) operators, which “create”/“annihilate”\(^1\) the single-particle state \( \beta \), while acting on the state of \( N \) indistinguishable particles, are defined by the following rules

\[ a^{+}_{\beta} \mid \alpha_1, \alpha_2, \ldots, \alpha_N \rangle = \sqrt{N} \langle \beta^{(1)} \mid \alpha_1, \alpha_2, \ldots, \alpha_N \rangle, \quad (1.12) \]

\[ a^{-}_{\beta} \mid \alpha_1, \alpha_2, \ldots, \alpha_N \rangle = \sqrt{N+1} S^{\!N}_{N+1} \{ \mid \beta \} \mid \alpha_1, \alpha_2, \ldots, \alpha_N \rangle, \quad (1.13) \]

where the state \( \mid \alpha_1, \alpha_2, \ldots, \alpha_N \rangle \) is the \( N \)-particle state defined as in Eq. (1.9).

Thus, in Eq. (1.12) the product is understood as the scalar product in the single-particle Hilbert space with the index \( i = 1 \) when the state of the indistinguishable particles is written as a linear combination of the states of identical particles, Eq. (1.9). Similar, the action of the projector \( S^{\!N}_{N+1} \) is defined by

\(^1\)This is exactly what their action means in the Fock space, see below.
employing the form of the state $|\alpha_1, \alpha_2, \ldots, \alpha_N\rangle$ given by Eq. (1.9) (where the single-particle state $|\beta\rangle$ occupies now the place with index $i = 1$, the state $|\alpha_1\rangle$ the place with index $i = 2$ and so on). We will frequently drop the superscript \(\varepsilon\) where it does not lead to a confusion.

Let us first study the action of the annihilation operator. First, we expand the symmetrization operator $S_N$ by employing the permutation, denoted below by $P_\ell$, which brings the $\ell$-th element of the ordered set $(1, 2, \ldots, N)$, to the first place while leaving the rest in the same order, i.e. acting as

$$P_\ell(1, 2, \ldots, N) = (\ell, 1, 2, \ldots, \ell - 1, \ell + 1, \ldots, N).$$

(1.14)

It has the signature equal to $\xi^{\ell-1}$, where $\xi = 1$ in the case of bosons and $\xi = -1$ in the case of fermions. We have the following property

$$S_N = \frac{1}{N} \sum_{\ell=1}^{N} \xi^{\ell-1} S^{[2, \ldots, N]}_{N-1} P_\ell,$$

(1.15)

where the projector $S^{[2, \ldots, N]}_{N-1}$ acts on the tensor product of the $N - 1$ single-particle states with the index varying from 2 to $N$. Thus we have

$$a_\beta^+ |\alpha_1, \alpha_2, \ldots, \alpha_N\rangle = \frac{1}{\sqrt{N}} \sum_{\ell=1}^{N} \xi^{\ell-1} \langle \beta | \alpha_{\ell} \rangle \underbrace{|\alpha_1\rangle \cdot \ldots \cdot |\alpha_{\ell-1}\rangle \cdot |\alpha_{\ell+1}\rangle \cdot \ldots \cdot |\alpha_N\rangle}_{\forall \alpha_{\ell}}.$$

(1.16)

Here and below the underbrace means that the state labelled by $\alpha_{\ell}$ is omitted from the expression for the $N$-particle state $|\alpha_1, \alpha_2, \ldots, \alpha_N\rangle$ making it a $(N-1)$-particle state (also of indistinguishable particles in this case).

On the other hand, using the obvious property $S_{N+1} S^{[2, \ldots, N+1]}_N = S_{N+1}$ (since $S^{[2, \ldots, N+1]}_N$ projects on the subspace of the projector $S_{N+1}$) we obtain from Eq. (1.13) the action of the creation operator as follows

$$a_\beta^{+} |\alpha_1, \alpha_2, \ldots, \alpha_N\rangle = \sqrt{\frac{N + 1}{N}} S^{[2, \ldots, N+1]}_{N+1} |\beta\rangle |\alpha_1\rangle |\alpha_2\rangle \cdots |\alpha_N\rangle.$$  

(1.17)

Note that expressions (1.16) and (1.17) make it evident that the resulting states belong to the respective physical Hilbert spaces, i.e. to $\mathcal{H}_{N-1}$ and $\mathcal{H}_{N+1}$, respectively.

Another useful representation of the action of the creation operator, which is used below, is given by expanding the symmetrization operator similar to Eq. (1.15), but using now the inverse operator $P_\ell^{-1}$ instead, i.e. which acts as

$$P_\ell^{-1}(1, 2, \ldots, N) = (2, \ldots, \ell - 1, \ell, 1, \ell + 1, \ldots, N),$$

where $P_1^{-1} = I$ since $P_1 = I$. With the use of $P_\ell^{-1}$ the $(N + 1)$-particle symmetrization operator is cast as

$$S_{N+1} = \frac{1}{N + 1} \sum_{\ell=1}^{N+1} \xi^{\ell-1} S^{[2, \ldots, N+1]}_{N} P_\ell^{-1}.$$
Using this property, we get

\[
\begin{align*}
a_\beta^+ | \alpha_1, \alpha_2, \ldots, \alpha_N \rangle &= \frac{1}{\sqrt{N+1}} \left[ | \beta^{(1)} \rangle | \alpha_1^{(2)}, \ldots, \alpha_N^{(N+1)} \rangle \
+ \sum_{\ell=1}^{N} \xi_\ell \sum_{\alpha_\ell} | \alpha_\ell^{(1)} \rangle | \alpha_1^{(2)}, \ldots, \alpha_N^{(N+1)} \rangle \right].
\end{align*}
\] (1.18)

Note that this expression resembles some features of that for the annihilation operator, Eq. (1.16).

Now, using the definitions of the creation and annihilation operators one can easily prove the following properties:

\[
\begin{align*}
(a_\pm)^\dagger &= a_\mp, \\
(1.19) \\
a_\pm a_\pm - \xi a_\mp a_\mp &= 0, \\
(1.20) \\
a_\pm^{-1} a_\pm - \xi a_\pm^{+} a_\pm &= \langle \gamma | \beta \rangle, \\
(1.21)
\end{align*}
\]

where \( \xi = 1 \) for bosons and \( \xi = -1 \) for fermions.

**Proof of the properties (1.19)-(1.21).** I. Consider property (1.19). We have

\[
\begin{align*}
\langle \beta_1, \ldots, \beta_{N+1} | a_\gamma^+ | \alpha_1, \ldots, \alpha_N \rangle^\dagger &= \langle \alpha_1, \ldots, \alpha_N | a_\gamma^- | \beta_1, \ldots, \beta_{N+1} \rangle.
\end{align*}
\]

Indeed, by the definition of the creation operator, Eq. (1.13), we have

\[
\begin{align*}
\langle \beta_1, \ldots, \beta_{N+1} | a_\gamma^+ | \alpha_1, \ldots, \alpha_N \rangle^\dagger &= \sqrt{N+1} \langle \gamma | \alpha_1, \ldots, \alpha_N \rangle \\
= \langle \alpha_1, \ldots, \alpha_N | a_\gamma^- | \beta_1, \ldots, \beta_{N+1} \rangle.
\end{align*}
\]

where we have used \( S_{N+1}^\dagger = S_{N+1}, \ S_{N+1}^2 = S_{N+1} \) and the definition of the annihilation operator, Eq. (1.12).

II. Consider now the property (1.20). Due to Eq. (1.16) we have

\[
\begin{align*}
a_\gamma^- a_\beta^- | \alpha_1, \ldots, \alpha_N \rangle &= a_\gamma^- \left( \frac{1}{\sqrt{N}} \sum_{\ell=1}^{N} \xi^{\ell-1} \langle \beta | \alpha_\ell \rangle | \alpha_1, \ldots, \alpha_N \rangle \right) \\
= \frac{1}{\sqrt{N-1}} \frac{1}{\sqrt{N}} \left( \sum_{\ell=1}^{N} \xi^{\ell-1} \sum_{m=1}^{N} \xi^{m-1} \langle \gamma_m | \beta \rangle \langle \alpha_m | \alpha_\ell \rangle | \alpha_1, \ldots, \alpha_N \rangle \right)
\end{align*}
\]
\begin{align*}
\sum_{\ell=1}^{N} \sum_{m=\ell+1}^{N} \xi^{m-2} \xi^{\ell-1} \langle \gamma \mid \alpha_m \rangle \langle \beta \mid \alpha_\ell \rangle |_{\forall \alpha_\ell \lor \alpha_m} \mid_{\alpha_1, \ldots, \alpha_N}^{-},
\end{align*}

where in the second and third lines the states labelled \( \alpha_\ell \) and \( \alpha_m \) are omitted from the state vector. By interchanging the indices \( \ell \) and \( m \) in the third line we obtain

\begin{align*}
a_\gamma^* a_\beta^* | \alpha_1, \ldots, \alpha_N \rangle = & \frac{1}{\sqrt{N-1}} \sum_{\ell=1}^{N} \sum_{m=1}^{\ell-1} \xi^{\ell+m-2} \left( \langle \gamma \mid \alpha_m \rangle \langle \beta \mid \alpha_\ell \rangle 
+ \xi \langle \gamma \mid \alpha_\ell \rangle \langle \beta \mid \alpha_m \rangle \right) |_{\forall \alpha_\ell \lor \alpha_m} \mid_{\alpha_1, \ldots, \alpha_N}^{-}.
\end{align*}

Property (1.20) for the annihilation operators evidently follows from Eq. (1.22). For the creation operators this property follows by application of property (1.19).

III. Consider the two sides of Eq. (1.21) applied to a state vector. We have

\begin{align*}
a_\gamma^* a_\beta^+ | \alpha_1, \ldots, \alpha_N \rangle = & \frac{1}{\sqrt{N+1}} \sum_{\ell=1}^{N} \sum_{m=1}^{\ell-1} \xi^{\ell+m-2} \left( \langle \gamma \mid \alpha_m \rangle \langle \beta \mid \alpha_\ell \rangle 
+ \xi \langle \gamma \mid \alpha_\ell \rangle \langle \beta \mid \alpha_m \rangle \right) |_{\forall \alpha_\ell \lor \alpha_m} \mid_{\alpha_1, \ldots, \alpha_N}^{-}.
\end{align*}

where we have used the property

\begin{align*}
S_{N+1} = \frac{1}{N+1} S_N^{[1, \ldots, N+1]} \left( I_{N+1} + \sum_{\ell=2}^{N+1} \xi P_{1\ell} \right),
\end{align*}

where \( P_{1\ell} \) is the operator corresponding to the permutation \( (1, \ell) \). On the other hand we have

\begin{align*}
a_\beta^* a_\gamma^* | \alpha_1, \ldots, \alpha_N \rangle = & \sum_{\ell=1}^{N} \xi^{\ell-1} \langle \gamma \mid \alpha_\ell \rangle S_N \{ | \beta \rangle \mid_{\alpha_1} \ldots \mid_{\alpha_N} \} 
= & \sum_{\ell=1}^{N} \langle \gamma \mid \alpha_\ell \rangle |_{\forall \alpha_\ell} \mid_{\alpha_1, \ldots, \alpha_N}^{-}.
\end{align*}

where we have used Eqs. (1.13) and (1.16) (in the last line the underbrace means the state labelled by \( \alpha_\ell \) is replaced by the one labelled by \( \beta \)). Comparing expressions (1.23) and (1.25) one arrives at property (1.21).

Since the creation and annihilation operators are, by Eq. (1.19), Hermitian conjugated to each other, we will adopt the notation \( a_\alpha \) for the annihilation operator, while the creation operator will be denoted by \( a_\alpha^\dagger \).
One easily verifies the following properties (valid for both types of particles, bosons and fermions):

\[ [a^\dagger_\alpha, a^\dagger_\beta] = \langle \alpha | \beta \rangle a^\dagger_\alpha, \quad [a_\alpha, a_\beta] = -\langle \beta | \alpha \rangle a_\alpha. \]  

(1.26)

An important property of the creation/annihilation operators, which is a direct consequence of their definitions, Eqs. (1.12) and (1.13), is that they depend linearly on the state which they “create”/“annihilate” (more precisely, the creation operator is linear in the state and the annihilation operator is anti-linear in the state, the latter is linear in the Hermitian conjugate state).

Writing explicitly the dependence of the creation/annihilation operators on the state, i.e.

\[ a^\dagger_\alpha \equiv A^+ (| \alpha \rangle), \quad a_\alpha \equiv A^- (\langle \alpha |), \]  

(1.27)

we have the following linearity property

\[ A^+ \left( \sum_j C_j | X_j \rangle \right) = \sum_j C_j A^+ (| X_j \rangle), \quad A^- \left( \sum_j D_j \langle X_j | \right) = \sum_j D_j A^- (\langle X_j |). \]  

(1.28)

This property allows the change of basis for the creation and annihilation operators, quite similarly as the change of basis is performed for the quantum states themselves. Indeed, expanding the state \( | \alpha \rangle \) in a basis \( | \alpha \rangle = \sum_j \langle j | \alpha \rangle | j \rangle \) we get

\[ a^\dagger_\alpha = \sum_j \langle j | \alpha \rangle a^\dagger_j, \quad a_\alpha = \sum_j \langle \alpha | j \rangle a_j. \]  

(1.29)

### 1.4 The Fock space

The linearity of the creation and annihilation operators on the “created” or “annihilated” state implies that it is sufficient to consider them for the orthogonal basis states. More importantly, their transformations between the basis states follow from those of the basis states themselves, as in Eq. (1.29). Only the number of particles in each single-particle state, comprising the \( N \)-particle state, is the most important parameter. Thus we have naturally come to the concept of the occupation number representation of the physical Hilbert space, i.e. to the concept of the Fock space. Suppose that we are given a basis in the Hilbert space \( H \) of the single-particle states

\[ | 1 \rangle, | 2 \rangle, | 3 \rangle, \ldots, | k \rangle, \ldots; \quad \langle k | j \rangle = \delta_{kj}. \]  

(1.30)

It is convenient to use the “variable index notation” for the basis states, which does not specify which particular \( N \) states of the basis are selected, i.e. for \( N \) particles we will write the basis state as \( | k_j \rangle \), with \( j = 1, 2, \ldots, N \) (here \( k_j \) is a natural number and some \( k_j \) with different \( j \) may coincide). The \( N \)-particle states for indistinguishable particles are given now as

\[ | k_1, k_2, \ldots, k_N \rangle = \frac{1}{N!} \sum_{P} \varepsilon(P) | k_{P^{-1}(1)} \rangle \cdot \ldots \cdot | k_{P^{-1}(N)} \rangle. \]  

(1.31)
The state defined by Eq. (1.31) is, in general, not normalized. One can define the normalized $N$-particle states for the indistinguishable particles, which we will call the Fock states. For bosons the normalized states are given as

$$| n_{k_1}, n_{k_2}, \ldots, n_{k_s} \rangle \equiv \left( \frac{N!}{n_{k_1}! n_{k_2}! \ldots n_{k_s}!} \right)^{\frac{1}{2}} | k_1, k_2, \ldots, k_N \rangle,$$

where we assume that only the states $k_j$, $j = 1, \ldots, s$ are occupied, while for fermions we can also write

$$| n_1, n_2, \ldots, n_N \rangle \equiv \sqrt{N!} | k_1, k_2, \ldots, k_N \rangle,$$

where due to the Pauli exclusion principle all $n_j = 1$. The numbers $n_j$ are called the occupation numbers (for fermions the occupation numbers $n_j$ take just two values 0 and 1). The normalizing factors in Eqs. (1.32) and (1.33) follow from the definition of the state $| k_1, k_2, \ldots, k_N \rangle$, Eq. (1.31), and simple calculation.

Let us consider the action of the creation and annihilation operators on the Fock states (1.32) and (1.33).

1. **Boson case.** We have (for simplicity, we rename $n_{k_j}$ into $n_k$)

$$a_{k_j} | n_{k_1}, \ldots, n_k \rangle = \left( \frac{N!}{n_{k_1}! \ldots n_k!} \right)^{\frac{1}{2}} a_{k_j} | k_1, k_2, \ldots, k_N \rangle$$

$$= \left( \frac{N!}{n_{k_1}! \ldots n_k!} \right)^{\frac{1}{2}} \frac{1}{\sqrt{N}} \sum_{l=1}^{N} \langle k_j | k_l \rangle | k_1, \ldots, k_N \rangle$$

$$= \left( \frac{(N - 1)!}{n_{k_1}! \ldots n_k!} \right)^{\frac{1}{2}} \sum_{k_l = k_j}^{N} | k_1, \ldots, k_N \rangle$$

$$= \sqrt{n_{k_j}} | n_{k_1}, \ldots, n_{k_j} - 1, \ldots, n_k \rangle,$$

where we have used Eq. (1.16) and the orthogonality of the single-particle basis vectors (the last summation is over all indices $k_l$ coinciding with $k_j$). Similarly

$$a_{k_j}^\dagger | n_{k_1}, \ldots, n_k \rangle = \left( \frac{N!}{n_{k_1}! \ldots n_k!} \right)^{\frac{1}{2}} \sqrt{N + 1} S_{N+1} \{ | k_j \rangle | k_1, k_2, \ldots, k_N \rangle \}$$

$$= \left( \frac{(N + 1)!}{n_{k_1}! \ldots (n_{k_j} + 1)! \ldots n_k!} \right)^{\frac{1}{2}} \sqrt{n_{k_j} + 1} | k_j, k_1, k_2, \ldots, k_N \rangle$$

$$= \sqrt{n_{k_j} + 1} | n_{k_1}, \ldots, n_{k_j} + 1, \ldots, n_k \rangle,$$

where we have used the definition, Eq. (1.13), and the symmetry property of the state vector for bosons.

---

2Due to the asymmetry with respect to the labels $k_j$, the fermion $N$-particle state depends on the order of the single-particle states in it, a swap of any two such states leads to a $\pi$-phase.
Let us also introduce the vacuum state, \( | \text{Vac} \rangle \), i.e. the state with no particles (\( N = 0 \)). It has the following property

\[
a_{k_j} | \text{Vac} \rangle = 0,
\]

(1.36)

for any annihilation operator \( a_{k_j} \) (and, due to the linearity property of the operator in the state it annihilates, Eq. (1.28), for arbitrary boson annihilation operator). Then, one can use Eq. (1.34) to represent the Fock basis state in the following form

\[
| n_{k_1}, n_{k_2}, \ldots, n_{k_N} \rangle = \frac{(a_{k_1}^\dagger)^{n_{k_1}} \cdots (a_{k_N}^\dagger)^{n_{k_N}}}{\sqrt{n_{k_1}! \cdots n_{k_N}!}} | \text{Vac} \rangle.
\]

(1.37)

**II. Fermion case.** In the fermion case, as different from the boson case, the order of the single-particle states in the \( N \)-particle state is important. Thus, the formulae derived above for bosons have their analogs for fermions with the additional phases due to transpositions used to add or remove the single-particle states to and from the \( N \)-particle one. Using Eq. (1.16) we have, for instance,

\[
a_{k_j} | n_{k_1}, n_{k_2}, \ldots, n_{k_N} \rangle = \frac{1}{\sqrt{N!}} \sum_{\ell=1}^{N} (-1)^{\sum_{m<j} n_{k_m}} \langle k_j | k_\ell \rangle | k_1, \ldots, k_N \rangle
\]

\[
= \delta_{n_{k_j}, 1} (-1)^{\sum_{i<j} n_{k_i}} | k_1, \ldots, k_N \rangle
\]

\[
= (-1)^{\sum_{i<j} n_{k_i}} \sqrt{n_{k_j}} | n_{k_1}, \ldots, n_{k_j} - 1, \ldots, n_{k_N} \rangle,
\]

(1.38)

where \( n_{k_m} \) is the occupation number of the \( k_m \) state. Similarly,

\[
a_{k_j}^\dagger | n_{k_1}, n_{k_2}, \ldots, n_{k_N} \rangle = \sqrt{N+1} A_{N+1}^{[2 \ldots N+1]} | k_j \rangle | n_{k_1}, n_{k_2}, \ldots, n_{k_N} \rangle
\]

\[
= \sqrt{(N+1)!} A_{N+1}^{[1]} | k_j \rangle | k_1 \rangle \cdots | k_N \rangle
\]

\[
= \delta_{n_{k_j}, 0} (-1)^{\sum_{i<j} n_{k_i}} \sqrt{(N+1)!} A_{N+1}^{[1]} | k_1 \rangle \cdots | k_j \rangle \cdots | k_N \rangle
\]

\[
= (-1)^{\sum_{i<j} n_{k_i}} \sqrt{n_{k_j} + 1} | n_{k_1}, \ldots, n_{k_j} + 1, \ldots, n_{k_N} \rangle,
\]

(1.39)

where we have used that \( A_{N+1}^{[2 \ldots N+1]} A_{N+1}^{[1]} = A_{N+1} \) and the fact that for \( n_{k_j} = 1 \) the state \( | n_{k_1}, \ldots, n_{k_j}, 1, \ldots, n_{k_N} \rangle \) becomes zero.

In the fermion case the Fock state (with all \( n_{k_j} = 1 \)) is given as

\[
| n_{k_1}, n_{k_2}, \ldots, n_{k_N} \rangle = \sqrt{N!} | k_1, k_2, \ldots, k_N \rangle = a_{k_1}^\dagger \cdots a_{k_N}^\dagger | \text{Vac} \rangle,
\]

(1.40)

where \( | \text{Vac} \rangle \) is the fermion vacuum state.

For the boson and fermion cases one can define the occupation-number operator as

\[
n_k = a_k^\dagger a_k,
\]

(1.41)
which gives the occupation number of the corresponding single-particle state (this operator is a scalar in the Fock space, thus we use the same notation).

Note that one can write down the unnormalized \( N \)-particle basis state of the indistinguishable particles for both, boson and fermion cases, as follows

\[
| k_1, k_2, \ldots, k_N \rangle = \frac{1}{\sqrt{N!}} a_{k_1}^\dagger \cdots a_{k_N}^\dagger | \text{Vac} \rangle,
\]

(1.42)

where in the boson case, some \( k_j \) with different index \( j \) may coincide. The importance of this representation will become clear below. The expansion of unit operator, i.e. the projector \( S_N \) on the physical Hilbert space of \( N \) indistinguishable particles now can be written as follows (for bosons and fermions)

\[
\sum_{\sum_j n_j = N} | n_1, n_2, \ldots, n_s, \ldots \rangle \langle n_1, n_2, \ldots, n_s, \ldots | = S_N,
\]

(1.43)

where the summation is over all sets of occupation numbers, such that their sum is \( N \). Moreover, due to the summation identity

\[
\sum_{\sum_j n_j = N} \frac{N!}{n_{k_1}!n_{k_2}! \cdots n_{k_N}!} \{ \ldots \} = \sum_{k_1} \cdots \sum_{k_N} \{ \ldots \},
\]

(1.44)

the same projector operator can be expressed using the unnormalized states as

\[
\sum_{k_1} \cdots \sum_{k_N} | k_1, k_2, \ldots, k_N \rangle \langle k_1, k_2, \ldots, k_N | = S_N,
\]

(1.45)

where the last formula has an important advantage for below, since the summations over the state indices \( k_j \) vary independently of each other.

### 1.5 The representations of state vectors and operators

#### 1.5.1 \( N \)-particle wave-functions

We did not specify the basis for construction of the Fock space and used only the orthogonality of the single-particle basis states. In this respect, the linearity of the creation and annihilation operators in the state they create or annihilate allows to pass from one Fock space to the other. For instance, assume that we pass from the basis of infinite but countable number states to the co-ordinate representation as follows (here the index \( k \) may include also the spin variable)

\[
| k \rangle = \int dx \varphi_k(x) | x \rangle,
\]

(1.46)

where \( \varphi_k(x) \equiv \langle x | k \rangle \) is the wave-function corresponding to the basis state \( | k \rangle \) and \( | x \rangle \) is the basis state in the co-ordinate representation. Denoting the
creation and annihilation operators of the co-ordinate basis state \( |x\rangle \) as \( \psi^\dagger(x) \) and \( \psi(x) \) by Eq. (1.28) we have

\[
    a_k^\dagger = \int dx \varphi_k(x) \psi^\dagger(x), \quad a_k = \int dx \varphi_k^*(x) \psi(x).
\]

(1.47)

The inverse transformation also follows from Eq. (1.28):

\[
    \psi(x) = \sum_k \varphi_k(x) a_k, \quad \psi^\dagger(x) = \sum_k \varphi_k^*(x) a_k^\dagger.
\]

(1.48)

In the same way as for the one-particle case, one can define the wave-function for the case of \( N \) indistinguishable particles. Indeed, one just need to project the Fock state (a multi-particle analog of the basis state \( |k\rangle \)) onto the expansion (1.45) of the unit operator in the physical space, i.e. the projector \( S_N \). Using the basis states from the co-ordinate representation (with the summation in Eq. (1.45) substituted by the integration over all coordinates) we define

\[
    \varphi(x_1, \ldots, x_N) \equiv \langle x_1, \ldots, x_N | n_{k_1}, \ldots, n_{k_s} \rangle,
\]

(1.49)

so that now

\[
    | n_{k_1}, \ldots, n_{k_s} \rangle = \int dx_1 \ldots \int dx_N \varphi(x_1, \ldots, x_N) | x_1, \ldots, x_N \rangle
\]

\[
    = \frac{1}{\sqrt{N!}} \int dx_1 \ldots \int dx_N \varphi(x_1, \ldots, x_N) \psi^\dagger(x_1) \cdot \ldots \cdot \psi^\dagger(x_N) | \text{Vac} \rangle,
\]

(1.50)

where we have used Eq. (1.42) now for the co-ordinate basis states of \( N \) indistinguishable particles. Thus one may even use the notation \( |\varphi_N\rangle \) for this Fock state. The scalar product between two \( N \)-particle wave-functions is given by the usual integral formula, again due to the property (1.45), i.e.

\[
    \langle \phi_N | \varphi_N \rangle = \int dx_1 \ldots \int dx_N \phi^*(x_1, \ldots, x_N) \varphi(x_1, \ldots, x_N),
\]

(1.51)

where the co-ordinates under the integrals vary independently. Hence, we have arrived at the “usual” \( N \)-particle wave-function representation for the state of \( N \) indistinguishable particles, which also can be obtained as appropriate symmetrization of the single-particle wave-functions. Indeed we have from the definitions (1.32) and (1.49)

\[
    \varphi(x_1, \ldots, x_N) = \langle x_1, \ldots, x_N | \left( \frac{N!}{n_{k_1}! n_{k_2}! \cdots n_{k_s}!} \right)^{\frac{1}{2}} S_N \{ |k_1\rangle \cdots |k_N\rangle \}
\]

\[
    = \left( \frac{N!}{n_{k_1}! n_{k_2}! \cdots n_{k_s}!} \right)^{\frac{1}{2}} S_N \{ \langle x_1 |k_1\rangle \cdots \langle x_N |k_N\rangle \}
\]

17
\[
\left( \frac{N!}{n_{k_1}!n_{k_2}!\cdots n_{k_s}!} \right)^{1/2} S_N \{ \varphi_{k_1}(x_1) \cdots \varphi_{k_s}(x_N) \},
\] (1.52)

where we have used the projector property \( S_N^2 = S_N \) allowing to remove the symmetrization from the basis vector \( \langle x_1, \ldots, x_N | \) before evaluation of the scalar product (note the normalizing factor in this definition).

## 1.5.2 The second-quantization representation of operators

The observables of the system of indistinguishable particles, the physical operators for below, are just the symmetric subset of all operators acting in the Hilbert space of identical (i.e. distinguishable) particles. Thus the physical operators can be expanded over the basis of the Hilbert space of identical particles. However, we will be interested in the representation of these in the physical subspace only, i.e. how they act over the space of indistinguishable particles. We will show that their action can be expressed as action of the products of the creation and annihilation operators.

**The one-particle operators.** Let us start with the one-particle operators (which act on the \( N \)-particle Hilbert space and should not be confused with single-particle ones). We have a general structure of such an operator

\[
A_1 = A^{(1)} + A^{(2)} + \ldots + A^{(N)},
\] (1.53)

where \( A^{(j)} \) is the single-particle operator acting on the Hilbert space of the \( j \)th particle. A one-particle operator (1.53) is symmetric as it should be for an observable describing a system of indistinguishable particles.

If we use two basis vectors of the single-particle Hilbert space, such that the matrix element of a single-particle operator is \( \langle \alpha | A^{(1)} | \beta \rangle \), the representation of a one-particle operator in the Hilbert space of identical particles has the form

\[
A_1 = \sum_\alpha \sum_\beta \langle \alpha | A^{(1)} | \beta \rangle \sum_{j=1}^N | \alpha^{(j)} \rangle \langle \beta^{(j)} |,
\] (1.54)

where the last summation is understood as a direct sum of the operators acting in the single-particle Hilbert spaces indexed from 1 to \( N \). The aim is find how a one-particle operator acts on the physical subspace. By Eq. (1.54) this amounts to finding out how the last sum acts in the physical subspace. The latter is given by the following identity

\[
\sum_j | \alpha^{(j)} \rangle \langle \beta^{(j)} | = a_\alpha^\dagger a_\beta,
\] (1.55)

valid in the physical space, i.e. the Hilbert space of indistinguishable particles. Indeed, let us prove it by analyzing how it acts on a \( N \)-particle state (of the indistinguishable particles) and comparing to the product of the operators on
the r.h.s. We have obviously
\[
\sum_{j=1}^{N} \left| \alpha^{(j)} \right\rangle \left\langle \beta^{(j)} \right| k_1, \ldots, k_N = \frac{1}{N} \sum_{j=1}^{N} \sum_{\ell=1}^{N} \xi^{j-1} \langle \beta | k_\ell \rangle S_{N-1}^{[1\ldots j-1,j+1\ldots N]} \left\{ \left| k_1^{(1)} \right\rangle \ldots \left| \alpha^{(j)} \right\rangle \ldots \left| k_N^{(N)} \right\rangle \right\} \right| k_\ell \rangle
\]
\[
= \sum_{\ell=1}^{N} \langle \beta | k_\ell \rangle \left| k_1, \ldots, k_N \right\rangle ,
\]
here we have used the factorization of the symmetrization operator \( S_N \) similar to Eq. (1.15) where instead the \( k_\ell \)th vector is brought not to the first but to the \( j \)th place. Comparing with Eq. (1.25) we get the result (1.55). Note that the r.h.s. of Eq. (1.55) does not depend on the number of particles, thus leading to a representation for the many-particle operator \( A_1 \) in Eq. (1.54) which is \( N \)-independent. We have in particular
\[
A_1 = \sum_{\alpha} \sum_{\beta} \langle \alpha | A^{(1)} | \beta \rangle a^\dagger \alpha a_\beta . \tag{1.56}
\]
Eq. (1.55) can also be shown using the following properties
\[
\xi^{j-1} \sqrt{\frac{N}{j}} \langle \beta^{(j)} | k_1, \ldots, k_N \rangle = a_\beta \left| k_1, \ldots, k_N \right\rangle ,
\]
\[
\frac{1}{\sqrt{\frac{N}{j}}} \sum_{j=1}^{N} \xi^{j-1} \left| \alpha^{(j)} \right\rangle \left| k_1, \ldots, k_N \right\rangle = a^\dagger \alpha \left| k_1, \ldots, k_N \right\rangle , \tag{1.57}
\]
where the first property follows from Eq. (1.16) noticing that \( \langle \beta^{(j)} | k_1, \ldots, k_N \rangle = \xi^{j-1} \langle \beta^{(1)} | k_1, \ldots, k_N \rangle \), while in the second it is understood that new vector occupies the \( j \)th place in the product of the single-particle vectors in the state \( \left| k_1, \ldots, k_N \right\rangle \) and we have used Eq. (1.17) and a factorization of the symmetrization operator similar to that of Eq. (1.15).

The many-particle operators. The generalization to the \( s \)-particle operators, acting in the Hilbert space of indistinguishable particles is obvious. We have
\[
A_s = \sum_{j_1 < j_2 < \ldots < j_s} A^{(j_1 \ldots j_s)} = \frac{1}{s!} \sum_{P} \sum_{j_1 < \ldots < j_s} A^{(P(j_1) \ldots P(j_s))} , \tag{1.58}
\]
where to satisfy the property of being an observable describing the system of indistinguishable particles, the operator \( A^{(j_1 \ldots j_s)} \) must be symmetric with respect to permutations of the indices \( j_1, \ldots, j_s \). Indeed, by definition of the physical observable, for any permutation \( P \) of the state of identical particles we must have
\[
\langle f_1^{(1)}, \ldots, f_N^{(N)} | A_s | k_1^{(1)}, \ldots, k_N^{(N)} \rangle = \langle f_1^{(1)}, \ldots, f_N^{(N)} | P^\dagger A_s P | k_1^{(1)}, \ldots, k_N^{(N)} \rangle ,
\]
19
i.e. \( P^\dagger A_s P = A_s \) and since \( P^\dagger A^{(j_1, \ldots, j_s)} P = A^{(P^{-1}(j_1), \ldots, P^{-1}(j_s))} \) (compare with Eq. (1.9)).

Let us now generalize Eq. (1.55) to the \( s \)-particle representation. We have

\[
\sum_{P} \sum_{j_1 < \ldots < j_s} | \alpha^{(j_1)}_{P(1)} \rangle \cdots | \alpha^{(j_s)}_{P(s)} \rangle | \beta^{(j_1)}_{P(1)} \rangle \cdots | \beta^{(j_s)}_{P(s)} \rangle = a^\dagger_{\alpha_1} \cdots a^\dagger_{\alpha_s} \beta_{\alpha_1} \cdots \beta_{\alpha_s},
\]

again, valid in the physical space, i.e. the Hilbert space of indistinguishable particles. To see why a permutation \( P \) must appear, note that the summation over the ordered indices \( j_1 < \ldots < j_s \) is lifted to the summation over the unequal indices \( j_1, \ldots, j_s \) by this permutation, while by Eq. (1.55) it is almost evident that the indices in the summation can indeed appear in an arbitrary order. Now, let us prove Eq. (1.59). To this end we compute how the r.h.s. of this equation acts on the state vector. We will use the following factorization of the symmetrization operator

\[
S_N = \frac{(N-s)!}{N!} \sum_{\ell_1 < \ldots < \ell_s} \prod_{\ell_k} \xi_{\ell_k} \prod_{P_s} \xi(P_s) P_s S_{N-s}^{[s+1, \ldots, N]},
\]

where a permutation of \( N \) elements is factorized into a product of the permutations \( P_s \) of the first \( s \) and the last \( N-s \) elements (summed up to the symmetrization operator \( S_{N-s}^{[s+1, \ldots, N]} \)) and a permutation between these two subsets (given by the summation over the ordered set of indices \( \ell_1, \ldots, \ell_s \)). By using Eq. (1.60) we obtain (the change of order in the annihilation operator indices is made for convenience of notations)

\[
A_{\beta_1} \cdots A_{\beta_s} | k_1, \ldots, k_N \rangle = [N(N-1) \cdots (N-s+1)]^{-\frac{1}{2}} \times \sum_{\ell_1 < \ldots < \ell_s} \prod_{\ell_k} \xi_{\ell_k} \prod_{P_s} \xi(P) \langle \beta_1 | k_{P(\ell_1)} \rangle \cdots \langle \beta_s | k_{P(\ell_s)} \rangle \langle k_1, \ldots, k_N \rangle.
\]

Now we must calculate how the creation operators of Eq. (1.59) act on this result. Applying consecutively the definition of the creation operator, Eq. (1.13), we get

\[
a^\dagger_{\alpha_1} \cdots a^\dagger_{\alpha_s} | k_1, \ldots, k_N \rangle \times S_N \{| \alpha^{(1)} \rangle \cdots | \alpha^{(s)} \rangle \langle k_1, \ldots, k_N \rangle \}_{\forall k_{\ell_1} \cdots \forall k_{\ell_s}}
\]

\[
= \sum_{\ell_1 < \ldots < \ell_s} \prod_{\ell_k} \xi_{\ell_k} \prod_{P_s} \xi(P) \langle \beta_1 | k_{P(\ell_1)} \rangle \cdots \langle \beta_s | k_{P(\ell_s)} \rangle \times S_N \{| \alpha^{(1)} \rangle \cdots | \alpha^{(s)} \rangle \langle k_1, \ldots, k_N \rangle \}_{\forall k_{\ell_1} \cdots \forall k_{\ell_s}}
\]

\[
= \sum_{\ell_1 < \ldots < \ell_s} \sum_P \langle \beta_{P^{-1}(1)} | k_{\ell_1} \rangle \cdots \langle \beta_{P^{-1}(s)} | k_{\ell_s} \rangle | k_1, \ldots, k_N \rangle \}_{k_{\ell_1} \rightarrow \alpha_{P^{-1}(1)}, \ldots, k_{\ell_s} \rightarrow \alpha_{P^{-1}(s)}},
\]

where we have transferred the permutation \( P \) to the indices of \( \beta \)'s and used the property \( PS_N = \xi(P) S_N \) to transfer the signature of this permutation to action.
of this permutation on \(\alpha\)-vectors. The final step is to note that the last line is exactly the action of the l.h.s. of Eq. (1.59) on the state vector.

Now let us expand the \(s\)-particle operator in the product of the single-particle basis states. We have

\[
A_s = \sum_{\alpha_1,\ldots,\alpha_s, \beta_1,\ldots,\beta_s} \sum_{j_1 < \ldots < j_s} |\alpha_1^{(j_1)}\rangle \ldots |\alpha_s^{(j_s)}\rangle A_s(\alpha_1,\ldots,\alpha_s|\beta_s,\ldots,\beta_1) \\
\times \langle\beta_s^{(j_s)}| \ldots \langle\beta_1^{(j_1)}|
\]

(1.61)

where the operator is represented by a symmetric function in the simultaneous permutation of both \(\alpha\)’s and \(\beta\)’s:

\[
A_s(\alpha_1,\ldots,\alpha_s|\beta_s,\ldots,\beta_1) \equiv \langle\alpha_1^{(1)}| \ldots \langle\alpha_s^{(s)}| A(1\ldots s) |\beta_s^{(s)}\rangle \ldots |\beta_1^{(1)}\rangle.
\]

Therefore, adding a summation over the permutations of \(s\) elements and using Eq. (1.59) we obtain

\[
A_s = \frac{1}{s!} \sum_{\alpha_1,\ldots,\alpha_s, \beta_1,\ldots,\beta_s} A_s(\alpha_1,\ldots,\alpha_s|\beta_s,\ldots,\beta_1) a_{\alpha_1}^\dagger \ldots a_{\alpha_s}^\dagger a_{\beta_s} \ldots a_{\beta_1}.
\]

(1.62)

One commentary on the identity (1.59) is in order. On the l.h.s. there is an operator which is not symmetrized in the indices \(\alpha\) or \(\beta\), whereas on the r.h.s. the operator is symmetrized, since by the commutation relations, we have

\[
Pa_{\alpha_1}^\dagger \ldots a_{\alpha_s}^\dagger = \xi(P)a_{\alpha_1}^\dagger \ldots a_{\alpha_s}^\dagger a_{\beta_1}^\dagger \ldots a_{\beta_s}^\dagger.
\]

In fact, due to this property of the r.h.s., one can apply the symmetrization to the vectors on the l.h.s. and obtain the following identity

\[
\sum_P \sum_{j_1 < \ldots < j_s} |\alpha_{P(1)},\ldots,\alpha_{P(s)}\rangle \langle\beta_{P(s)},\ldots,\beta_{P(1)}| = a_{\alpha_1}^\dagger \ldots a_{\alpha_s}^\dagger a_{\beta_s} \ldots a_{\beta_1},
\]

(1.63)

where the vectors on the l.h.s. are composed as symmetrized products of the vectors from the single-particle spaces with the indices \(j_1,\ldots,j_s\).

### 1.5.3 Examples

Consider the (one-dimensional) position and momentum operators of a system of \(N\) indistinguishable particles. The observables formed of these two single-particle operators must be symmetric with respect to permutation of the particles, thus the only form they have is that of a sum:

\[
X = \frac{1}{N} \sum_{j=1}^N x^{(j)}, \quad P = -i\hbar \sum_{j=1}^N \frac{\partial}{\partial x^{(j)}},
\]

(1.64)

where we have used that the total momentum is a sum of the momenta of all the particles and defined a the coordinate to be canonically conjugate to the momentum operator, i.e. \([P,X] = -i\hbar\). Let us find the “second-quantized”
form of this operators. Define the creation and annihilation operators of the 
co-ordinate state $|x\rangle$ as $\psi^\dagger(x)$ and $\psi(x)$. Then, the form of the one-particle 
operators $X$ and $P$ is given by Eq. (1.56) (the summation is replaced by the 
integration):

\[
X = \frac{1}{N} \int dx \, x \psi^\dagger(x)\psi(x), \quad P = \int dx \, \psi^\dagger(x) \left( -i\hbar \frac{\partial}{\partial x} \right) \psi(x),
\]  
(1.65)

where, to arrive at the second formula, we have used that $\langle x' | \frac{\partial}{\partial x} | x \rangle = -\frac{\partial}{\partial x} \delta(x' - x)$ and used the integration by parts. To clarify what physical entity corresponds 
to the position observable $X$ notice that the number of particles is given by the 
following formula

\[
N = \int dx \psi^\dagger(x)\psi(x).
\]  
(1.66)

Hence $\rho(x) \equiv \psi^\dagger(x)\psi(x)$ is the operator of the density of particles at $x$ (i.e. the 
average density is $\langle S | \rho(x) | S \rangle$, for a state $|S\rangle$) and $\rho(x)/N$ gives the probability 
density to find a particle at this point. Therefore, $X$ indeed describes the 
distribution of position of the particles in the system.

Consider now a system of $N$ indistinguishable particles interacting by some 
forces. We have in this case the Hamiltonian

\[
H = -\frac{\hbar^2}{2m} \sum_{j=1}^{N} \frac{\partial^2}{\partial r^{(j)} \partial r^{(j)}} + \sum_{1 \leq i < j \leq N} U(|r^{(i)} - r^{(j)}|).
\]  
(1.67)

Using Eq. (1.62) we get for the interaction potential (the integration $\int d^3r(...)$ 
is over the volume)

\[
\sum_{1 \leq i < j \leq N} U(|r^{(i)} - r^{(j)}|) = \frac{1}{2} \int d^3r \int d^3r' U(|r - r'|) \psi^\dagger(r) \psi^\dagger(r') \psi(r) \psi(r'),
\]

which has a clear physical meaning, since the integrand is almost $\frac{1}{2} U(|r - r'|) \rho(r) \rho(r')$ (except for the auto-interaction term $-\frac{1}{2} U(|r-r'|) \delta(r-r') \psi^\dagger(r') \psi(r')$), which describes the interaction of a concentration of particles at $r$ with that at $r'$ by the potential $U(|r - r'|)$ with the account of the indistinguishability given 
by the coefficient $\frac{1}{2}$. Hence, the Hamiltonian reads

\[
H = \int d^3r \psi^\dagger(r) \left( -\frac{\hbar^2}{2m} \nabla^2 \right) \psi(r) + \frac{1}{2} \int d^3r \int d^3r' U(|r - r'|) \psi^\dagger(r) \psi^\dagger(r') \psi(r') \psi(r).
\]  
(1.68)

1.6 Evolution of operators in the Heisenberg picture

Before we present the evolution of the creation and annihilation operators, let us 
show the following useful identity about the commutator in the case of fermions.
We have

\[ [A, B_1 B_2 \cdots B_{2n}] = \{A, B_1\} B_2 \cdots B_{2n} - B_1 \{A, B_2\} B_3 \cdots B_{2n} + \ldots + (-1)^{2n-1} B_1 \cdots B_{2n-1} \{A, B_{2n}\}, \]

where \( \{A, B\} = AB + BA \) is the anti-commutator. This identity can be verified by induction. Since in the number of particle preserving Hamiltonian the number of creation and annihilation fermion operators is the same, the above identity allows one to expand the commutator \([H, A]\) using the anti-commutators of \(A\) with the creation and annihilation operators. We will use then the unified notation \([A, B]_\xi\) which denotes the commutator in the case of bosons and anti-commutator in the case of fermions, with this notation and the replacement of \(-1\) by \(\xi\) the above identity becomes universally valid for bosons and fermions:

\[ [A, B_1 B_2 \cdots B_{2n}] = \{A, B_1\} B_2 B_3 \cdots B_{2n} + \xi B_1 \{A, B_2\} B_3 B_4 \cdots B_{2n} + \ldots + \xi^{2n-1} B_1 B_2 \cdots B_{2n-1} \{A, B_{2n}\}, \]

(1.69)

In the Heisenberg picture, the evolution is transferred to the observables, i.e. we have the operator equation

\[ i\hbar \frac{\partial}{\partial t} A = [A, H], \]

(1.70)

where \(A\) is any observable of the quantum system and \(H\) is its Hamiltonian. Let us use Eq. (1.70) for the annihilation operator \(\psi(r)\) for the system of indistinguishable particles with the Hamiltonian given by Eq. (1.68). Using Eq. (1.69) to compute the commutators:

\[ [\psi(r), \psi^\dagger(r_1)] \left( -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial r_1^2} \psi(r_1) \right) = [\psi(r), \psi^\dagger(r_1)]_\xi \left( -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial r_1^2} \psi(r_1) \right) \]

\[ + \xi [\psi^\dagger(r_1)] \left( -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial r_1^2} \psi(r_1) \right) = -\delta(r - r_1) \frac{\hbar^2}{2m} \frac{\partial^2}{\partial r_1^2} \psi(r_1), \]

where we have used the linearity of the commutator (to apply the linear operator \(\frac{\partial^2}{\partial r_1^2}\) after the evaluation of the commutator itself) and the commutation rules of the creation and annihilation operators, and

\[ [\psi(r), \psi^\dagger(r_1) \psi^\dagger(r_2) \psi(r_2) \psi(r_1)] = \delta(r - r_1) \psi^\dagger(r_2) \psi(r_2) \psi(r_1) + \xi \delta(r - r_2) \psi^\dagger(r_1) \psi(r_2) \psi(r_1) \]

\[ = [\delta(r - r_1) \psi^\dagger(r_2) \psi(r_2) + \delta(r - r_1) \psi^\dagger(r_1) \psi(r_1)] \psi(r), \]

where we have used the commutation rules of the creation and annihilation operators (e.g. the two annihilation operators in the second term on the r.h.s. we replaced in the second line). Using these results we obtain from Eqs. (1.70) and (1.68) the following evolution equation for the annihilation operator

\[ i\hbar \frac{\partial}{\partial t} \psi(r) = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial r^2} \psi(r) + \left( \int d^3r' U(|r - r'|) \psi^\dagger(r') \psi(r') \right) \psi(r). \]

(1.71)
Note that the second term defines a common potential for the particles through the particle density operator \( \rho(r) = \psi^\dagger(r)\psi(r) \), i.e.

\[
U(r) = \int d^3r' \rho(r') U(|r-r'|), \tag{1.72}
\]
so that the evolution equation may be cast in the form resembling that of the usual Schrödinger equation

\[
i\hbar \frac{\partial}{\partial t} \psi(r) = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial r^2} \psi(r) + U(r) \psi(r). \tag{1.73}
\]

This is one of the reasons the method is sometimes called the second quantization (one can say that we have performed the “second quantization” of the Schrödinger equation to arrive at Eq. (1.73)).

### 1.7 Statistical operators of indistinguishable particles

The method of statistical operators was developed by N.N. Bogoliubov [1]. Suppose that we describe a system of \( N \gg 1 \) indistinguishable particles and are interested in the \( s \)-particle operators, with \( s \) being much less than \( N \) (usually, \( s = 1 \) or \( 2 \)). Being interested in the few-particle observables, instead of using the full \( N \)-particle state of the system (or the full density matrix) one can use the so-called statistical operators of particle complexes (or the statistical operators of Bogoliubov) which fully describe the properties of such observables. For simplicity we assume that the \( N \)-particle system is in the pure state \( |\Psi_N\rangle \) (using the density matrix is a straightforward generalization). Expanding it in the physical basis, i.e.

\[
|\Psi_N\rangle = \sum_{\{n_l\}} \Phi_{\{n_l\}} |\{n_l\}\rangle, \tag{1.74}
\]

where the set \( \{n_l\} \) is the corresponding set of occupation numbers of the basis state. The \( s \)-particle statistical operator is given by the partial trace of the symmetrized (i.e. physical) state of Eq. (1.74) over the \( N-s \) single-particles Hilbert spaces, i.e.

\[
\mathcal{R}_s \equiv \text{Tr}_{s+1,...,N} \left( |\Psi_N\rangle \langle \Psi_N| \right)
= \sum_{k_{s+1}} \cdots \sum_{k_N} \left[ \langle k_{s+1}^{(s+1)} | \cdots | k_N^{(N)} \right] \langle \Psi_N | \langle \Psi_N | \left[ \left| k_{s+1}^{(s+1)} \right\rangle \cdots \left| k_N^{(N)} \right\rangle \right], \tag{1.75}
\]

where the vectors \( | k_j \rangle \) are the orthogonal basis states in the single-particle Hilbert space. Due to the property of the symmetrization operators \( S_N S_{N-s} = S_N \) one can use in Eq. (1.75) the (unnormalized) symmetrized basis vectors instead. Moreover, one can use the identity given by Eq. (1.43), but now for the \( N-s \) particles, to arrive at the following more simple expression of the
statistical operator (with the drawback, however, that the notations do not indicate over which single-particle spaces the inner product is taken)

\[ R_s = \sum_{\{\tilde{n}_l\}} \langle \{\tilde{n}_l\} | \Psi_N \rangle \langle \Psi_N | \{\tilde{n}_l\} \rangle, \quad (1.76) \]

where \( \{\tilde{n}_l\} \) is the normalized symmetrized vector made of \( \{|k^{(s+1)}_1\ldots k^{(N)}_N\rangle\).

In the special case, when the state of the system is one of the basis states, \( |\Psi_N\rangle = |\{n_l\}\rangle \), one can derive an insightful explicit expression for the \( s \)-particle operator. In this case, the \( s \)-particle operator of Eq. (1.75) can be cast as follows

\[ R_s = \sum_{\sum m_l = s} \frac{\prod C_{n_l}^{m_l}}{C_N^s} | \{m_l\} \rangle \langle \{m_l\} |, \quad (1.77) \]

where \( C_n^k = \frac{n!}{(n-k)!k!} \) is the usual combinatorial coefficient and the vector \( |\{m_l\}\rangle \) is the short-hand notation for a state of \( s \) particles with the occupation numbers \( m_l \leq n_l \), with \( n_l \) being the occupation numbers of the system state. This result is valid for both bosons and fermions, in the latter case, however, one can drop the combinatorial coefficient in the numerator since it is equal to 1 (and all the occupation numbers \( m_l \) are also equal to either 0 or 1). Note that the physical meaning of the scalar factor in Eq. (1.77) is the probability of finding \( s \) particles exactly in the state \( |\{m_l\}\rangle \langle \{m_l\}| \), where the particles/states are drawn from the state of the system \( |\{n_l\}\rangle \). Indeed, let us show that the sum of these coefficients (probabilities) is exactly 1. This follows from the following identity

\[(x + y)^N = \prod_l (x + y)^{n_l} = \prod_l \left( \sum_{m_l = 0}^{n_l} C_{n_l}^{m_l} x^{m_l} y^{n_l - m_l} \right) = \sum_{\{m_l\}} \prod_l C_{n_l}^{m_l} \sum y_l \sum (n_l - m_l).\]

Taking the partial derivative, i.e. applying the operator \( \frac{1}{s!} \frac{1}{(N-s)!} \frac{\partial^s}{\partial x^s} \frac{\partial^{N-s}}{\partial y^{N-s}} \) at \( (x = 0, y = 0) \) we get

\[ \frac{N!}{s!(N-s)!} = \sum_{\sum m_l = s} \prod_l C_{n_l}^{m_l}, \]

where \( \sum_l n_l = N. \)

To arrive at the explicit expression for the \( s \)-particle statistical operator (1.77), we will use the property of the symmetrization operator given by Eq. (1.60). We have then

\[ R_s = \frac{N!}{\prod_l n_l!} \left( \frac{(N-s)!}{N!} \right)^2 \sum_{l_1 < \ldots < l_s} \prod_{\ell_l} \xi^{\ell_l - 1} \sum_{\ell_1 < \ldots < \ell_k} \prod_{\ell_k} \xi^{\ell_k - 1} \sum_{P_j} \xi(P_j) \sum_{P_j'} \xi(P_j') \]
\[
\prod_{l} (m_l - n_l)! \prod_{l} \delta_{m_l, n_l} \sum_{s} \prod_{l} \xi(P_{s}) \sum_{P_{s}} \xi(P') \sum_{P_{s}} \sum_{m_l - n_l} \prod_{l} \left( \frac{s!}{m_l! (m_l - n_l)!} \right)^{s} \prod_{l} \frac{1}{(n_l - m_l)!} \sqrt{C_{N} C_{N}'} \left| \{ m_l \} \right> \left< \{ m_l' \} \right|
\]

where we have used Eq. (1.60) to rewrite each basis vector \(| f_1, \ldots, f_N \rangle\) from the expansion of the system state \(| \Psi_N \rangle\) in the following form

\[
| f_1, \ldots, f_N \rangle = \frac{(N - s)!}{N!} \prod_{l} \xi^{l-1} \sum_{P_{s}} \xi(P_{s}) \sum_{P_{s}} \xi(P') \sum_{P_{s}} \sum_{m_l} \prod_{l} \left( \frac{s!}{m_l! (m_l - n_l)!} \right)^{s} \prod_{l} \frac{1}{(n_l - m_l)!} \sqrt{C_{N} C_{N}'} \left| \{ m_l \} \right> \left< \{ m_l' \} \right|
\]

and introduced the normalized vectors \(| \{ m_l \} \rangle\) and \(| \{ n_l - m_l \} \rangle\)

\[
| \{ m_l \} \rangle = \left( \frac{s!}{\prod_{l} m_l!} \right)^{\frac{1}{2}} S_{s} \left| f_{l_1} \right> \left< f_{l_s} \right|
\]

\[
| \{ n_l - m_l \} \rangle = \left( \frac{(N - s)!}{\prod_{l} (n_l - m_l)!} \right)^{\frac{1}{2}} S_{N-s} \left| f_{l_{s+1}} \right> \left< f_{l_N} \right|
\]

corresponding to the partition of a set \((f_1, \ldots, f_N)\) into \((f_{l_1}, \ldots, f_{l_s})\) and \((f_{l_{s+1}}, \ldots, f_{l_N})\).

Taking the trace as in Eq. (1.76) is equivalent to setting \(n_l = n_l - m_l\) and multiplying by the inverse of the corresponding normalization factor \(\prod_{l} (n_l - m_l)!/(N - s)!\).

Now using in Eq. (1.78) the following summation identity

\[
\sum_{l_1 < \ldots < l_s} (\ldots) = \sum_{\{m_l\}} \prod_{l} \frac{m_l!}{m_l! (m_l - n_l)!} (\ldots),
\]

and the fact that in the case of fermions the partitions of \(f\)'s and \(g\)'s should be the same (due to the delta-symbol in Eq. (1.78), in this case the signature \(\xi_{k-1}\) appears twice and cancels out) and in the case of bosons \(\xi = 1\), by rewriting the vectors in the normalized form, we get Eq. (1.77).

It is now quite clear that in the general case, when the \(N\)-particle state is a linear combination of the Fock-basis states Eq. (1.74). In this case, the \(s\)-particle statistical operator can be cast in the following form

\[
R_s = \sum_{\{n_l\}} \sum_{\{n_l'\}} \Phi^* (\{n_l'\}) \Phi (\{n_l\}) \sum_{\sum m_l = s} \sum_{\sum m_l' = s} \prod_{l} \left( \frac{\delta_{n_l - m_l, n_l' - m_l}}{\sqrt{C_{N} C_{N}'}} \right) \left| \{ m_l \} \right> \left< \{ m_l' \} \right|
\]

26
or by setting \( p_{l} \equiv n_{l} - m_{l} = n'_{l} - m'_{l} \) and using that \( C^{m_{l}}_{n_{l}} = C^{p_{l}}_{n_{l}} \) we get

\[
\mathcal{R}_{s} = \sum_{\{n_{l}\}} \sum_{\{n'_{l}\}} \Phi^{*}(\{n_{l}\})\Phi(\{n'_{l}\}) \sum_{l} \frac{\prod_{l} \sqrt{C_{n_{l}}^{p_{l}} C_{n'_{l}}^{p_{l}}}}{C_{N}^{s}} | \{n_{l} - p_{l}\} \rangle \langle \{n'_{l} - p_{l}\} |,
\]

(1.79)

where if \( p_{l} > \min(n_{l}, n'_{l}) \) the corresponding term is simply zero.

There is yet another general representation for the \( s \)-particle statistical operator, which follows directly from Eq. (1.79). Indeed, each vector in the product in Eq. (1.79) can be represented by action of the annihilation operator to the corresponding basis vector, i.e.,

\[
\prod_{l} \sqrt{C_{n_{l}}^{p_{l}} | \{n_{l} - p_{l}\} \rangle \langle \{n_{l}\} |},
\]

(in the case of fermions the product of the annihilation operators is ordered one, however, since there is a bra-vector in Eq. (1.79) the order does not matter) thus we have Eq. (1.79) rewritten in the form

\[
\mathcal{R}_{s} = \frac{1}{C_{N}^{s}} \sum_{\{n_{l}\}} \sum_{\{n'_{l}\}} \Phi^{*}(\{n'_{l}\})\Phi(\{n_{l}\}) \sum_{l} \frac{\prod_{l} \sqrt{p_{l}!}}{p_{l}!} | \{n_{l}\} \rangle \langle \{n'_{l}\} | (a_{l}^{\dagger})^{p_{l}},
\]

(1.80)

where the order of the creation is inverse to the order of the annihilation operators. The general result is thus given by the following simple formula

\[
\mathcal{R}_{s} = \frac{1}{C_{N}^{s}} \sum_{\{n_{l}\}} \sum_{l} \frac{a_{l}^{p_{l}} \rho_{N} (a_{l}^{\dagger})^{p_{l}}}{p_{l}!}.
\]

were \( \rho_{N} \) is the general \( N \)-particle density matrix (in our case \( \rho_{N} = | \Psi_{N} \rangle \langle \Psi_{N} | \)) and, in the case of fermions, the order of the operators on the left and on the right of it is inverse to each other.

### 1.7.1 The averages of the \( s \)-particle operators

The average of the \( s \)-particle operator is defined as the trace of it with the state vector (or density matrix, in general). We have

\[
\langle A_{s} \rangle \equiv \text{Tr} \{ A_{s} | \Psi_{N} \rangle \langle \Psi_{N} | \}.
\]

(1.81)

We have using the expansion of the operator unit in the physical space, Eq. (1.45),

\[
\langle A_{s} \rangle = \sum_{k_{1}} \cdots \sum_{k_{N}} \langle k_{1}, \ldots, k_{N} | A_{s} | \Psi_{N} \rangle \langle \Psi_{N} | k_{1}, \ldots, k_{N} \rangle
\]

\[
= C_{N}^{s} \sum_{k_{1}} \cdots \sum_{k_{N}} \langle k_{1}, \ldots, k_{N} | A^{(1, \ldots, s)} | \Psi_{N} \rangle \langle \Psi_{N} | k_{1}, \ldots, k_{N} \rangle,
\]

(1.82)
where we have used the symmetry properties of the physical vectors and the symmetry property of the s-particle operator, i.e. $A^{(P^{-1}(1),...,P^{-1}(s))} = P^{t}A^{(1,...,s)}P$ and the number of all partitions $C_{N}^{s}$ of the set $(1,...,N)$ into $(j_{1},...,j_{s})$ and its complementary subset. Taking into account the definition of the s-particle statistical operator, Eq. (1.76), we get finally

$$\langle A_{s} \rangle = C_{N}^{s}\text{Tr}\{A^{(1,...,s)}\mathcal{R}_{s}\}. \quad (1.83)$$

Indeed, we have to verify that the partition of the summation in Eq. (1.82) into two subsets, using Eq. (1.60),

$$\langle k_{1},...,k_{N} \rangle = \frac{1}{C_{N}^{s}} \sum_{j_{1}<...<j_{s}} \prod_{l} \xi^{j_{l}-1} \langle k_{j_{1}},...,k_{j_{s}} \mid \langle k_{j_{s+1}},...,k_{j_{N}} \rangle \rangle \quad (1.84)$$

leads to Eq. (1.83). But this is evident from the following considerations. First, by the symmetry with respect to the permutations of s elements in $A^{(1,...,s)}$ and the symmetry properties of the physical vectors we get

$$\langle k_{j_{1}},...,k_{j_{s}} \rangle \langle k_{j_{s+1}},...,k_{j_{N}} \rangle \mid A^{(1,...,s)} \mid \Psi_{N} \rangle = [(\langle k_{j_{1}} \mid \ldots \langle k_{j_{N}} \mid ) A^{(1,...,s)} \mid \Psi_{N} \rangle,

\langle \Psi_{N} \mid k_{j_{1}},...,k_{j_{N}} \rangle = \langle \Psi_{N} \mid k_{j_{s+1}},...,k_{j_{N}} \rangle].$$

Second, by noticing that the summation over the ordered set $l_{1}<...<l_{s}$ gives exactly the $C_{N}^{s}$ equal terms, which cancels the coefficient $1/C_{N}^{s}$ in Eq. (1.84) (for the fermion case, the signature cancels out too since the single-particle states $|k_{j}\rangle$ used to build the N-particle state are all different). We arrive then at Eq. (1.83).

Consider now the particular choice of the s-particle operator given through the s-partition of the co-ordinate basis vectors $|x_{1},...,x_{N}\rangle$ (we consider the one-dimensional case for the simplicity of formulae below) as follows

$$X_{s} = \sum_{j_{1}<...<j_{s}} S_{s}\{[x_{1}^{(j_{1})},...,x_{s}^{(j_{s})}]S_{s}\{[\tilde{x}_{1}^{(j_{1})},...,\tilde{x}_{s}^{(j_{s})}]\}]. \quad (1.85)$$

Obviously, $X_{s}$ is a symmetric operator, hence an observable in the physical space. Then by Eq. (1.63) we get a simpler representation for $X_{s}$:

$$X_{s} = \frac{1}{s!} \psi^{\dagger}(x_{1}) \cdot \ldots \cdot \psi^{\dagger}(x_{s})\psi(\tilde{x}_{s}) \cdot \ldots \cdot \psi(\tilde{x}_{1}). \quad (1.86)$$

On the other hand, by using Eqs. (1.83) with $A_{s} = X_{s}$ and Eq. (1.85) we obtain the identity

$$\langle X_{s} \rangle = C_{N}^{s}\mathcal{R}_{s}(\tilde{x}_{1},...,\tilde{x}_{s} \mid x_{1},...,x_{s}) = C_{N}^{s}\mathcal{R}_{s}(\tilde{x}_{1},...,\tilde{x}_{s} | x_{1},...,x_{s}).$$

Therefore, we have arrived at the important identity for the s-particle statistical operator in the co-ordinate representation:

$$\mathcal{R}_{s}(\tilde{x}_{1},...,\tilde{x}_{s} | x_{1},...,x_{s}) = \frac{(N-s)!}{N!} \langle \psi^{\dagger}(x_{1}) \cdot \ldots \cdot \psi^{\dagger}(x_{s})\psi(\tilde{x}_{s}) \cdot \ldots \cdot \psi(\tilde{x}_{1}) \rangle. \quad (1.87)$$
Finally, by using the co-ordinate version of the general representation of a s-particle operator, Eq. (1.62), one can express the average of the s-particle observable also as follows

\[
\langle A_s \rangle = \frac{1}{s!} \int dx_1 \cdots \int dx_s \int d\tilde{x}_1 \cdots \int d\tilde{x}_s A_s(\tilde{x}_1, \ldots, \tilde{x}_s|x_1, \ldots, x_s) \\
\times \langle \psi^\dagger(x_1) \cdots \psi^\dagger(x_s)\psi(\tilde{x}_s) \cdots \psi(\tilde{x}_1) \rangle.
\]

By comparing with Eq. (1.83) we again obtain the result of Eq. (1.87).

When the total number of particles in the system is not fixed it is more convenient to work with the non-normalized statistical operators. First of all, the notion of the statistical operator \( R_s \) can be easily generalized to such systems. Indeed, one observes observing that \( R_s \) is linear in the state of the system, i.e. if the system is described by the density matrix \( \rho = \sum_N p_N \rho_N, 0 \leq p_N \leq 1 \)

then \( R_s = \sum_N p_N R_s^{(N)} \), where each \( R_s^{(N)} \) is defined for \( \rho_N \) by Eq. (1.75) with \( |\Psi_N\rangle \langle \Psi_N| \) substituted by \( \rho_N \).

Note that, for instance, the diagonal part of the 1-particle statistical operator \( R_1 \) in the co-ordinate representation is proportional to the density \( R_1(r|r) = N^{-1} \langle \psi^\dagger(r)\psi(r) \rangle \), thus it is convenient to introduce the operator \( \sigma_1 \) by \( \sigma_1(r'|r) = N R_1(r'|r') = \langle \psi^\dagger(r)\psi(r') \rangle \) which does not involve the total number of particles directly and is applicable to the systems with variable number of particles. The s-particle statistical operator \( \sigma_s \) can be thus defined through the \( R_s \) by the following formula

\[
\sigma_s = \sum_N p_N \frac{N!}{(N-s)!} R_s^{(N)},
\]

or, using Eq. (1.87), we get in the coordinate representation (in the three dimensions now)

\[
\sigma_s(\tilde{r}_1, \ldots, \tilde{r}_s|\tilde{r}_1, \ldots, \tilde{r}_s) = \langle \psi^\dagger(\tilde{r}_1) \cdots \psi^\dagger(\tilde{r}_s)\psi(\tilde{r}_s) \cdots \psi(\tilde{r}_1) \rangle.
\]

1.7.2 The general structure of the one-particle statistical operator

Consider a system of \( N \) indistinguishable particles in a pure state (1.74), i.e.

\[
|\Psi_N\rangle = \sum_{\{n_1\}} \Phi_{\{n_1\}}|\{n_1\}\rangle.
\]

The goal is to find the general expression for the one-particle statistical operator \( R_1 \). We will use the expression (1.80), i.e.

\[
R_1 = \frac{1}{N} \sum_i \sum_{m_i=N-1} \prod_{l} a_{\downarrow l}^{m_i} |\Psi_N\rangle \langle \Psi_N| (a_{\downarrow l}^{\dagger})^{m_i}.
\]
We have here

\[
\prod_{\{i: \sum m_i = N-1\}} \frac{a_i^{m_i}}{m_i!} \langle n_i \rangle \langle \tilde{n}_i \rangle | a_i^{m_i} \rangle = \sum_{l_1, l_2} \sqrt{n_l \tilde{n}_l} \langle f_{l_1} \rangle \langle f_{l_2} |,
\]

where the occupation number \( n_l \) corresponds to the state \( | f_l \rangle \) (in the case of bosons \( n_l \geq 1 \) and for fermions \( n_l = 1 \)). Since we also “remove” equal number of particles from each \( l \)-th state in the bra and ket vectors, there are just two cases: i) there is such \( l = \ell \) that \( m_\ell = n_\ell - 1 \), while for \( l \neq \ell \) \( m_l = n_l \), and the same is true for \( \tilde{n}_l \) and ii) there are two such \( l_1 \) and \( l_2 \) that \( m_{l_1} = n_{l_1} - 1 \) and \( m_{l_2} = n_{l_2} - 1 = n_{l_2} \). Depending on the \( N \)-particle state, we have a number of occurrences of both these cases in the one-particle operator \( \mathcal{R}_1 \). Therefore, using the formula (1.80) we obtain the following general structure of the one-particle operator \( \mathcal{R}_1 \):

\[
\mathcal{R}_1 = \sum_{l} \sum_{n=1}^{N} A^{(1)}_l (n) \frac{n}{N} | f_l \rangle \langle f_l | + \sum_{l_1 \neq l_2} \sum_{n_1, n_2=1}^{N} A^{(2)}_{l_1, l_2} (n_1, n_2) \frac{\sqrt{n_1 n_2}}{N} | f_{l_1} \rangle \langle f_{l_2} |,
\]

with the coefficients given by the formulae

\[
A^{(1)}_l (n) = \sum_{\{n, \ldots, n_l = n, \ldots\}} | \Phi(n_1, \ldots, n_l = n, \ldots)^2 |
\]

\[
A^{(2)}_{l_1, l_2} (n_1, n_2) = \sum_{\{n, \ldots, n_{l_1} = n_1 - 1, \ldots, n_{l_2} = n_2, \ldots\}} \Phi^*(n_1, \ldots, n_{l_1} = n_1 - 1, \ldots, n_{l_2} = n_2, \ldots)
\times \Phi(n_1, \ldots, n_{l_1} = n_1, \ldots, n_{l_2} = n_2 - 1, \ldots),
\]

where the summation is understood over all \( n_j \) except for the selected indices.

The obvious property \( (A^{(2)}_{l_1, l_2} (n_1, n_2))^* = A^{(2)*}_{l_2, l_1} (n_2, n_1) \) guarantees that the statistical operator is Hermitian, as it should be. Moreover, it is easy to verify that it has the unit trace, since

\[
\sum_{l} \sum_{n=1}^{N} A^{(1)}_l (n) \frac{n}{N} = \sum_{\{n, \ldots\}} \left( \sum_{l} \frac{n_l}{N} \right) | \Phi(n_1, \ldots, n_l, \ldots) \|^2 = 1.
\]

Finally, the non-normalized statistical operator \( \sigma_1 \) is given by the following formula

\[
\sigma_1 = \sum_{l} \sum_{n} A^{(1)}_l (n) | f_l \rangle \langle f_l | + \sum_{l_1 \neq l_2} \sum_{n_1, n_2} A^{(2)}_{l_1, l_2} (n_1, n_2) \sqrt{n_1 n_2} | f_{l_1} \rangle \langle f_{l_2} |,
\]

\[
= \sum_{l} \langle a_l^\dagger a_l | f_l \rangle \langle f_l | + \sum_{l_1 \neq l_2} \sum_{n_1, n_2} \langle a_{l_2}^\dagger a_{l_1} | f_{l_1} \rangle \langle f_{l_2} |.
\]

This representation clarifies the meaning of the eigenvalues of the Hermitian operator \( \sigma_1 \): they are the average occupation numbers of the corresponding eigenstates used as a Fock basis states, i.e. in the above representation, for instance, we have \( \langle n_l \rangle = \sum_n A^{(1)}_l (n) n \) by the definition of \( A^{(1)}_l (n) \).
Chapter 2

Quadratic Hamiltonian and the diagonalization

The properties of the Hamiltonians quadratic in the creation and annihilation operators are reviewed. The action of such a Hamiltonian is related to the canonical transformation, which is given in the explicit form. In the case of fermions the quadratic Hamiltonian can always be diagonalized by a unitary transformation. In the case of bosons the problem of diagonalization of a quadratic Hamiltonian is related to the old problem of stability of a solution to a Hamiltonian system of the classical mechanics, for instance, the notion of the Krein index plays also a crucial role for the diagonalization of the bosonic Hamiltonian. A simple criterion, i.e. a necessary and sufficient condition, to the latter problem is unknown, however, a sufficient condition for a quadratic bosonic Hamiltonian to be diagonalizable is the positivity or negativity of the related classical Hessian. Also, the diagonalization of a quadratic boson Hamiltonian in the case of a simplest (i.e. rank 2) zero mode is considered.
2.1 Diagonalization of the Hamiltonian quadratic in the fermion operators

The general form of a quadratic Hamiltonian operator is the following

\[ H = \sum_{\mu\nu} A_{\mu\nu} a_\mu a_\nu + \frac{1}{2} \sum_{\mu\nu} B_{\mu\nu} a_\mu a_\nu - \frac{1}{2} \sum_{\mu\nu} B_{\mu\nu}^* a_\mu^* a_\nu^*. \]  \hfill (2.1)

Here the indices run from 1 to \( N \) and, due to the fermion anti-commutation relations \( \{ a_\mu, a_\nu \} = 0 \) and \( \{ a_\mu, a_\nu^* \} = \delta_{\mu,\nu} \), the matrices satisfy the properties \( A^* = A \) and \( \tilde{B} = -B \), where the tilde denotes the matrix transposition, i.e. \( \tilde{B}_{\mu\nu} = B_{\nu\mu} \). Let us define the operator-valued columns and rows, i.e.:

\[
\begin{bmatrix}
a_1 \\
a_2 \\
\vdots \\
a_N
\end{bmatrix}, \quad \begin{bmatrix}
a_1 \\
a_2 \\
\vdots \\
a_N
\end{bmatrix}^* \equiv (a_1, a_2, \ldots, a_N), \tag{2.2}
\]

and similar the column \( a^\dagger \) and row \( \tilde{a}^\dagger \). Using the anti-commutators relations and that \( \tilde{A} = A^* \) we obtain

\[ \tilde{a}^\dagger A a = -\tilde{a} \tilde{A} a^\dagger + \text{Tr}(A) = -\tilde{a} A^* a^\dagger + \text{Tr}(A). \]

Hence, we can rewrite the Hamiltonian (2.1) in the following matrix form

\[ H = \frac{1}{2} \left( \begin{array}{cc} a_1 \\
a_2 \\
\vdots \\
a_N \end{array} \right) \left( \begin{array}{cc} A & B^\dagger \\
B & -A^* \end{array} \right) \left( \begin{array}{c} a \\\na^\dagger \end{array} \right) + \frac{1}{2} \text{Tr}(A). \tag{2.3} \]

Note the properties of the traceless matrix \( \mathcal{H} \) of the fermionic quadratic form (2.3):

\[ \mathcal{H} \equiv \left( \begin{array}{cc} A & B^\dagger \\
B & -A^* \end{array} \right), \quad \mathcal{H}^\dagger = \mathcal{H}, \quad \tau \mathcal{H} \tau = -\mathcal{H}^*, \quad \tau \equiv \left( \begin{array}{cc} 0 & I_{N\times N} \\
I_{N\times N} & 0 \end{array} \right), \tag{2.4} \]

i.e. \( \tau \) is the block off-diagonal matrix, where each block has the dimension \( N\times N \). The matrix \( \mathcal{H} \) could be a Hessian of a classical Hamiltonian system (with a quadratic Hamiltonian) if it were not for the minus sign at the last property (due to the anti-commutation relations between the fermion operators). We however will call \( \mathcal{H} \) the Hessian of a fermionic Hamiltonian. The analogy with the classical Hamiltonian system is possible for the bosonic quadratic Hamiltonian, considered in the next section.

We are interested in the possibility of diagonalizing of the Hamiltonian (2.3). Such a transformation, if it exists, must preserve the anti-commutation relations between the new fermion operators. A general linear transformation between the creation and annihilation operators can be put in the following form

\[ \begin{bmatrix} a \\ a^\dagger \end{bmatrix} = \begin{bmatrix} U & V^* \\ V & U^* \end{bmatrix} \begin{bmatrix} b \\ b^\dagger \end{bmatrix} = S \begin{bmatrix} b \\ b^\dagger \end{bmatrix}, \tag{2.5} \]
where the matrices $U$ and $V$ are to be constrained by the anti-commutations of the involved operators. We have

$$\{a_\mu, a_\nu\} = \sum_{\alpha, \beta} \{ U_{\mu \alpha} b_\alpha + V^*_{\mu \alpha} b_\alpha^\dagger, U_{\nu \beta} b_\beta + V^*_{\nu \beta} b_\beta^\dagger \} = \sum_{\alpha} (U_{\mu \alpha} V^*_{\nu \alpha} + V^*_{\mu \alpha} U_{\nu \alpha}) = 0,$$

$$\{a_\mu, a_\dagger_\nu\} = \sum_{\alpha, \beta} \{ U_{\mu \alpha} b_\alpha + V^*_{\mu \alpha} b_\alpha^\dagger, U^*_{\nu \beta} b_\beta^\dagger + V_{\nu \beta} b_\beta \} = \sum_{\alpha} (U_{\mu \alpha} U^*_{\nu \alpha} + V_{\mu \alpha} V^*_{\nu \alpha}) = \delta_{\mu, \nu},$$

i.e., in the matrix form, we have obtained the relations

$$UU^\dagger + V^*\tilde{V} = I, \quad UV^\dagger + V^*\tilde{U} = 0.$$  \hspace{1cm} (2.6)

These conditions, in their turn, guarantee also the existence of the inverse transformation to that of Eq. (2.5), i.e.,

$$\left( \begin{array}{c} b \\ b^\dagger \end{array} \right) = \left( \begin{array}{cc} U^\dagger & V^\dagger \\ \tilde{V} & \tilde{U} \end{array} \right) \left( \begin{array}{c} a \\ a^\dagger \end{array} \right) = S^\dagger \left( \begin{array}{c} a \\ a^\dagger \end{array} \right),$$  \hspace{1cm} (2.7)

due to the identities of Eq. (2.6) and the derivatives from those, which lead to the matrix identity

$$\left( \begin{array}{cc} U & V^* \\ V & U^* \end{array} \right) \left( \begin{array}{cc} U^\dagger & V^\dagger \\ \tilde{V} & \tilde{U} \end{array} \right) = \left( \begin{array}{cc} I & 0 \\ 0 & I \end{array} \right).$$  \hspace{1cm} (2.8)

By interchanging the order in the product of the matrices in Eq. (2.8), we obtain also the following relations

$$U^\dagger U + V^\dagger V = I, \quad \tilde{U} V + \tilde{V} U = 0,$$  \hspace{1cm} (2.9)

which are equivalent to the relations (2.6).

The unitary matrix $S$ which gives a canonical transformation must also satisfy the following property $\tau S \tau = S^*$, see Eq. (2.5). Hence there is such matrix $\Omega$ that

$$S = \left( \begin{array}{cc} U & V^* \\ V & U^* \end{array} \right) = e^{\iota \Omega}, \quad \Omega^\dagger = \Omega, \quad \tau \Omega \tau = -\Omega^*. \hspace{1cm} (2.10)$$

This is the most general form of a linear canonical transformation of the fermion creation and annihilation operators.

Let us now consider what constraints on the transformation (2.5) imposes diagonalization by this of the Hamiltonian (2.3). First of all, we must obtain

$$H = \sum_\mu \lambda_\mu b_\mu^\dagger b_\mu + \frac{\text{Tr}(A)}{2} \equiv \tilde{b}^\dagger \Lambda \tilde{b}, \quad \Lambda = \text{diag}(\lambda_1, \ldots, \lambda_N) + \frac{\text{Tr}(A)}{2}. \hspace{1cm} (2.11)$$

Then, calculating the commutators with the fermionic operators, we have

$$[a_\mu, H] = \sum_\nu (A_{\mu \nu} a_\nu - B^*_{\mu \nu} a^\dagger_\nu), \quad [a_\dagger_\mu, H] = \sum_\nu (-A^*_{\mu \nu} a_\nu + B_{\mu \nu} a^\dagger_\nu),$$
i.e., in the matrix form
\[
[a, H] = Aa - B^*a^\dagger, \quad [a^\dagger, H] = (-A^*a^\dagger + Ba).
\] (2.12)

On the other hand, using the transformation and the form of the Hamiltonian (2.11), we have
\[
[a, H] = [Ub + V^*b^\dagger, H] = UAb - V^*Ab^\dagger,
\]
\[
[a^\dagger, H] = [U^*b^\dagger + Vb, H] = VAb - U^*Ab^\dagger.
\] (2.13)

Expressing the \(a\)-operators through \(b\)-ones in the r.h.s. of Eq. (2.12), using the r.h.s. of Eq. (2.13) and the linear independence of the creation and annihilation operators\(^1\) we arrive at the eigenvalue problem for the Hessian matrix (2.4):
\[
\begin{pmatrix}
A & B^\dagger \\
B & -A^*
\end{pmatrix}
\begin{pmatrix}
U & V^* \\
V & U^*
\end{pmatrix}
= 
\begin{pmatrix}
\Lambda & 0 \\
0 & -\Lambda
\end{pmatrix}.
\] (2.14)

It is seen that the diagonalization problem always has a solution, since the Hessian is Hermitian (hence the real eigenvalues) while its properties guarantee that the eigenvalues always come in pairs \((\lambda_\mu, -\lambda_\mu)\) and the relation between the eigenvectors implied in Eq. (2.14) holds. Indeed, consider the eigenvector \(|\lambda_\mu\rangle\) corresponding to the eigenvalue \(\lambda_\mu \neq 0\). Due to properties (2.4) and that \(\tau^2 = I\) we have:
\[
\mathcal{H} |\lambda_\mu\rangle = \lambda_\mu |\lambda_\mu\rangle, \quad \mathcal{H} (\tau |\lambda_\mu\rangle) = -\lambda_\mu (\tau |\lambda_\mu\rangle),
\] (2.15)
which is precisely the relation expressed in Eq. (2.14) between the eigenvectors, i.e.
\[
|\lambda_\mu\rangle = \begin{pmatrix} U_\mu \\ V_\mu \end{pmatrix}, \quad |\lambda_\mu\rangle = \begin{pmatrix} V^*_\mu \\ U^*_\mu \end{pmatrix}.
\]

The above consideration could fail when the eigenvalue is equal to zero. However, since the non-zero eigenvalues come in pairs and the Hessian matrix is traceless (see Eq. (2.3)), an even number of linearly independent eigenvectors corresponds to zero eigenvalue. In the case when two (or any other, necessarily even number) of them satisfies the property \(\tau |X\rangle = \pm |X\rangle\) one can take the vectors \(|Z_+\rangle = |X\rangle \pm i |Y\rangle\) which satisfy the required property \(\tau |Z_+\rangle^* = |Z_-\rangle\), needed for the unitary transformation \(S\), diagonalizing the Hessian, to be also a canonical one.

Consider now the quantum evolution described by a fermionic quadratic Hamiltonian
\[
\hat{H} = \frac{1}{2} \begin{pmatrix} \bar{a}^\dagger & \bar{a} \end{pmatrix} \begin{pmatrix} E & F^\dagger \\
F & -E^* \end{pmatrix} \begin{pmatrix} a \\ a^\dagger \end{pmatrix},
\] (2.16)

\(^1\)One can see this fact by employing the inner products with the Fock space vectors \(|0\rangle\) and \(|1\rangle\) for each mode \(j = 1, \ldots, N\), i.e. \( \langle 0 | a_j \rangle = 1 \) while \( \langle 0 | a^\dagger_j \rangle = 0 \).

\(^2\)For notational convenience, we will use the Dirac notations also for the eigenvectors of matrices: the vector-columns will be the ket-vectors and the vector-rows – the bra-vectors.
where \( E^\dagger = E \) and \( \tilde{F} = -F \) as required. In the Heisenberg picture, the evolution by a unitary operator \( U(t) = e^{-i\hat{H}/\hbar} \) is transferred to the creation and annihilation operators, i.e.

\[
\begin{align*}
\mathbf{a}(t) &= e^{i\hat{H}/\hbar} \mathbf{a} e^{-i\hat{H}/\hbar}, \\
\mathbf{a}^\dagger(t) &= e^{i\hat{H}/\hbar} \mathbf{a}^\dagger e^{-i\hat{H}/\hbar},
\end{align*}
\tag{2.17}
\]

which is obviously also a canonical transformation. Moreover, it is also a linear canonical transformation and can be put in the form of Eq. (2.5). To arrive at the required transformation matrix, let us use by the well-known identity

\[
e^{B} \mathbf{A} e^{-B} = \sum_{p} \frac{[B, [B, \ldots, [B, A] \ldots]]}{p!},
\tag{2.18}
\]

where \( [B, A]^{(p)} \equiv [B, [B, \ldots, [B, A] \ldots]] \) is the successive commutator of \( B \) with \( A \) of order \( p \). We must compute the successive commutators of the Hamiltonian \( \hat{H} \) with the creation and annihilation operators \( a_\mu, a_\mu^\dagger \). By using the property of commutator of fermionic operator with an even number of operators, Eq. (1.69) of section 1.6, we obtain

\[
\begin{align*}
[\hat{H}, a_\mu] &= \sum_\nu (-E_{\mu\nu} a_\nu + F_{\mu\nu} a_\nu^\dagger), \\
[\hat{H}, a_\mu^\dagger] &= \sum_\nu (E_{\mu\nu} a_\nu^\dagger - F_{\mu\nu} a_\nu).
\end{align*}
\]

Writing \( \mathbf{A} = (a_1, \ldots, a_N, a_1^\dagger, \ldots, a_N^\dagger) \) and \( \hat{\mathbf{\hat{H}}} = \sum_{n,\ell} \hat{\mathbf{\hat{H}}}_{n\ell} \mathbf{A}_{n} \mathbf{A}_{\ell} \), where \( \hat{\mathbf{\hat{H}}} \) is the Hessian of the Hamiltonian (2.16),

\[
\hat{\mathbf{\hat{H}}} \equiv \begin{pmatrix} E & F^\dagger \\ F & -E^* \end{pmatrix},
\tag{2.19}
\]

we have

\[
[\hat{\mathbf{\hat{H}}}, \mathbf{A}_{n}] = -\sum_\ell \hat{\mathbf{\hat{H}}}_{n\ell} \mathbf{A}_{\ell}, \quad [\hat{\mathbf{\hat{H}}}, [\hat{\mathbf{\hat{H}}}, \mathbf{A}_{n}]] = \sum_\ell \hat{\mathbf{\hat{H}}}_{n\ell} \sum_m \hat{\mathbf{\hat{H}}}_{\ell m} \mathbf{A}_{m}, \ldots,
\]

i.e. we get

\[
[\hat{\mathbf{\hat{H}}}, \mathbf{A}_{n}]^{(p)} = \sum_\ell \left\{ (-\hat{\mathbf{\hat{H}}})^p \right\}_{n\ell} \mathbf{A}_{\ell}
\]

which implies that

\[
\begin{pmatrix} \mathbf{a}(t) \\ \mathbf{a}^\dagger(t) \end{pmatrix} = e^{i\hat{H}/\hbar} \begin{pmatrix} \mathbf{a} \\ \mathbf{a}^\dagger \end{pmatrix} e^{-i\hat{H}/\hbar} = e^{-i\hat{H}/\hbar} \begin{pmatrix} \mathbf{a} \\ \mathbf{a}^\dagger \end{pmatrix}.
\tag{2.20}
\]

The r.h.s. of this equation gives a linear canonical transformation by the properties of the Hessian \( \hat{\mathbf{\hat{H}}} \) (cf. with Eq. (2.10)). By comparing Eqs. (2.20) and (2.10) we see that a canonical transformation linear in the creation and annihilation operators can be expressed as a result of a temporal evolution given by another quadratic Hamiltonian with the Hessian provided by the exponential representation of the transformation as in Eq. (2.10): \( \hat{\mathbf{\hat{H}}} = \hbar \mathbf{\Omega} \) (for \( t = 1 \)).
2.2 Diagonalization of the Hamiltonian quadratic in the boson operators

Let us start with considering the quantum evolution governed by a Hamiltonian quadratic in bosonic operators,

\[ \hat{H} = \frac{1}{2} \begin{pmatrix} \tilde{a}_1^\dagger & \tilde{a} \end{pmatrix} \begin{pmatrix} E & F^* \\ F & E^* \end{pmatrix} \begin{pmatrix} a \\ a^\dagger \end{pmatrix}. \]

Here we have used the bosonic commutation relations to see that a general quadratic Hamiltonian,

\[ \hat{H} = \sum_{\mu\nu} E_{\mu\nu} a^\dagger_\mu a_\nu + \frac{1}{2} \sum_{\mu\nu} F_{\mu\nu} a_\mu a_\nu + \frac{1}{2} \sum_{\mu\nu} F^*_{\mu\nu} a^\dagger_\mu a^\dagger_\nu, \]

features \( E^\dagger = E \) and \( \tilde{F} = F \) and, by using

\[ \tilde{a}^\dagger E a = \tilde{a} E a^\dagger - \text{Tr}(E) = \tilde{a} E^* a^\dagger - \text{Tr}(E), \]

after dropping a scalar \(-\text{Tr}(E)/2\), can be cast in the form of Eq. (2.21). First, note that the Hessian matrix associated with the Hamiltonian (2.21) satisfies the usual properties of a Hessian of a classical Hamiltonian system:

\[ \hat{H} \equiv \begin{pmatrix} E & F^* \\ F & E^* \end{pmatrix}, \quad \hat{H}^\dagger = \hat{H}, \quad \tau \hat{H} \tau = \hat{H}^*. \]

This analogy is essential for the below discussed diagonalization of quadratic bosonic Hamiltonian.

Consider the unitary evolution operator \( \mathcal{U}(t) = e^{-i\hat{H}/\hbar} \) which, in the Heisenberg picture, induces a canonical transformation

\[ a(t) = e^{i\hat{H}/\hbar} a e^{-i\hat{H}/\hbar}, \quad a^\dagger(t) = e^{i\hat{H}/\hbar} a^\dagger e^{-i\hat{H}/\hbar}. \]

Similarly as in the fermion case, writing \( \mathcal{A} = (a_1, \ldots, a_N, a^\dagger_1, \ldots, a^\dagger_N) \) and \( \hat{H} = \sum_{n,\ell} \hat{H}_{n\ell} a_n a_\ell \), we compute the successive commutators \([\hat{H}, a_n]\) and arrive at the relation

\[ [\hat{H}, a_n]^p = \sum_{\ell} \{ (-J \hat{H})^p \}_{n\ell} a_\ell, \quad J \equiv \begin{pmatrix} I_{N \times N} & 0 \\ 0 & -I_{N \times N} \end{pmatrix}, \]

i.e. \( J \) is the block diagonal matrix, where each block has the dimension \( N \times N \). Thus, using Eq. (2.18) we obtain the identity

\[ \begin{pmatrix} a(t) \\ a^\dagger(t) \end{pmatrix} = e^{i\hat{H}/\hbar} \begin{pmatrix} a \\ a^\dagger \end{pmatrix} e^{-i\hat{H}/\hbar} = e^{-iJ\hat{H}/\hbar} \begin{pmatrix} a \\ a^\dagger \end{pmatrix}. \]

We will see below that, similar to the fermion case, the matrix on the r.h.s. of this equation, with the Hessian of the form of Eq. (2.22), gives a canonical
transformation linear in bosonic operators. Note that in the bosonic case, as distinct from the fermionic one, the unitary operator evolution is expressed by the transformation with a non-unitary matrix (hence the possibility of instabilities in the Hamiltonian dynamics describing the bosonic quasiparticles).

Let us now return to the diagonalization problem. First of all, consider a general linear transformation of the bosonic operators

$$\begin{pmatrix} a & a^\dagger \end{pmatrix} \equiv \begin{pmatrix} U & V^* \\ V & U^* \end{pmatrix} \begin{pmatrix} b & b^\dagger \end{pmatrix} = S \begin{pmatrix} b & b^\dagger \end{pmatrix}. \quad (2.25)$$

The commutation relations then give the following constraints

$$[a_\mu, a_\nu] = \sum_{\alpha,\beta} [U_{\mu\alpha} b_\alpha + V_{\mu\alpha} b_\alpha^\dagger, U_{\nu\beta} b_\beta + V_{\nu\beta} b_\beta^\dagger] = \sum_\alpha (U_{\mu\alpha} V_{\nu\alpha}^* - V_{\mu\alpha} U_{\nu\alpha}) = 0,$n

$$[a_\mu, a_\nu^\dagger] = \sum_{\alpha,\beta} [U_{\mu\alpha} b_\alpha + V_{\mu\alpha} b_\alpha^\dagger, U_{\nu\beta} b_\beta + V_{\nu\beta} b_\beta^\dagger] = \sum_\alpha (U_{\mu\alpha} U_{\nu\alpha}^* - V_{\mu\alpha} V_{\nu\alpha}) = \delta_{\mu,\nu},$$

i.e., in the matrix form, we have obtained the relations

$$UU^\dagger - V^* \tilde{V} = I, \quad UV^\dagger - V^* \tilde{V} = 0. \quad (2.26)$$

These conditions also guarantee the existence of the inverse transformation to that of Eq. (2.25), in this case we have (cf. with Eq. (2.7))

$$\begin{pmatrix} b & b^\dagger \end{pmatrix} = \begin{pmatrix} U^\dagger & -V^\dagger \\ -\tilde{V} & \tilde{U} \end{pmatrix} \begin{pmatrix} a & a^\dagger \end{pmatrix} = JS^\dagger J \begin{pmatrix} a & a^\dagger \end{pmatrix}. \quad (2.27)$$

Eq. (2.27) can be verified by using the identities (2.26) and the ones derived from those, which lead to

$$\begin{pmatrix} U & V^* \\ V & U^* \end{pmatrix} \begin{pmatrix} U^\dagger & -V^\dagger \\ -\tilde{V} & \tilde{U} \end{pmatrix} = \begin{pmatrix} I & 0 \\ 0 & I \end{pmatrix}, \quad (2.28)$$

i.e. $S^{-1} = JS^\dagger J$. By interchanging the order of the matrices in the product in Eq. (2.27) we obtain also

$$U^\dagger U - V^* \tilde{V} = I, \quad \tilde{V} V - \tilde{V} U = 0. \quad (2.29)$$

Note that the relations (2.29) are equivalent to those of Eq. (2.26), i.e. one set of relations leads to the other.

Note the following property of the bosonic canonical transformation (2.25), the matrix $U$ is invertible, i.e. $\det(U) \neq 0$. Indeed, the first relation in Eq. (2.29) excludes the possibility of non-trivial vectors in the kernel of matrix $U$, since $U|x\rangle = 0$ leads to a contradiction: $0 > -\langle x|V^\dagger V|x\rangle = \langle x|x\rangle > 0$. This is in contrast to the fermion case, where both $U$ and $V$ can be zero (the trivial exchange of the creation and annihilation operators is an example of a canonical transformation in the fermionic case).
Let us show that any canonical transformation (2.25) can be represented in the same form as on the r.h.s. of Eq. (2.24), thus proving that any linear canonical transformation can be represented by a unitary evolution with some quadratic Hamiltonian, exactly as in the fermion case. To this end we have to show that the transformation matrix $S$ of Eq. (2.25) can be cast in the exponential form, that is

$$S = \begin{pmatrix} U & V^* \\ V & U^* \end{pmatrix} = e^{-iJ\hat{H}},$$

(2.30)

with some matrix $\hat{H}$, i.e. having the properties of a Hessian: $\hat{H}^\dagger = \hat{H}$ and $\tau\hat{H}\tau = \hat{H}^\ast$. But the latter properties, together with the identity $J\tau = -\tau J$, are precisely the properties which guarantee that $\tau S\tau = S^\ast$, i.e. the right form of matrix $S$ as on the l.h.s. of Eq. (2.30), and $S^{-1} = JS^\dagger J$, Eq. (2.28), which is equivalent to the transformation being canonical, i.e. the conditions (2.26) being satisfied. Moreover, one can easily verify by direct calculation that the canonical transformations (2.25) form a group, i.e. a composition of two canonical transformations is also a canonical transformation.

Consider now the problem of diagonalization of a quadratic bosonic Hamiltonian

$$H = \sum_{\mu\nu} A_{\mu\nu} a^\dagger_{\mu} a_{\nu} + \frac{1}{2} \sum_{\mu\nu} B_{\mu\nu} a^\dagger_{\mu} a_{\nu} + \frac{1}{2} \sum_{\mu\nu} B^\ast_{\mu\nu} a_{\mu} a^\dagger_{\nu} + \frac{1}{2} \text{Tr}(A),$$

(2.31)

where $A^\dagger = A$ and $B^\dagger = B$, as required. By the same procedure as in the fermionic case, i.e. by using the commutation relations and the diagonalized form of the Hamiltonian (2.31),

$$H = \sum_{\mu} \lambda_{\mu} b^\dagger_{\mu} b_{\mu} + K \equiv \tilde{B}^\dagger \Lambda b + K, \quad \Lambda = \text{diag}(\lambda_1, \ldots, \lambda_N),$$

(2.32)

where $K$ is a scalar constant due to the non-commutation of the creation and annihilation operators (it will be computed below), we obtain the following equations

$$AU + B^\ast V = U\Lambda, \quad BU + A^\ast V = -V\Lambda.$$  

(2.33)

These lead to a non-Hermitian eigenvalue problem with the eigenvectors being the columns of the canonical transformation diagonalizing the Hamiltonian (2.31):

$$J\mathcal{H} \begin{pmatrix} U & V^* \\ V & U^* \end{pmatrix} = \begin{pmatrix} U & V^* \end{pmatrix} \begin{pmatrix} \Lambda & 0 \\ 0 & -\Lambda \end{pmatrix},$$

(2.34)

where $J$ is defined above Eq. (2.24), while $\mathcal{H}$ is the Hessian of the Hamiltonian, i.e.

$$\mathcal{H} = \begin{pmatrix} A & B^\ast \\ B & A^\ast \end{pmatrix}.$$  

(2.35)
First of all, the eigenvalue problem for the matrix $JH$, where $H$ is Hermitian and satisfies the property $\tau H \tau = H^*$ is related to the linear stability problem of a classical Hamiltonian system whose Hessian at the solution to be studied for stability is exactly $H$ (see below). Let us discuss some properties of the eigenvalue problem (2.35). The eigenvalues come in quartets $\{\lambda_\mu, -\lambda_\mu, \lambda_\mu^*, -\lambda_\mu^*\}$. This is easily seen from the properties of $H$ and that $J\tau = -\tau J$:

$$JH \langle X | \rangle = \lambda \langle X | \rangle, \quad JH (\tau | X\rangle^*) = -\lambda^* (\tau | X\rangle^*) , \quad (2.36)$$

while from the existence of the left-eigenvector $\langle Y | JH = \lambda \langle Y |$ we get

$$JH (J | Y\rangle) = \lambda^* (J | Y\rangle), \quad JH (\tau J | Y\rangle^*) = -\lambda (\tau J | Y\rangle^*) .$$

The inner product which corresponds to the normalization condition of the eigenvectors, required by the canonical transformation, i.e. $U^\dagger U - V^\dagger V = I$, where we use $| X_\mu \rangle = (U_\mu, V_\mu)^T$, must be defined as $\langle X_\mu | J | X_\nu \rangle$ and is indefinite. The other condition of Eq. (2.29) is the orthogonality condition in this inner product between the eigenvectors corresponding to different eigenvalues, i.e. the eigenvectors $| X_\mu \rangle$ corresponding to $\lambda_\mu$ and $\tau | X_\nu \rangle^*$ corresponding to $-\lambda_\nu$.

The eigenvectors corresponding to the eigenvalues $\lambda_1$ and $\lambda_2$ are orthogonal if $\lambda_2 \neq \lambda_1^*$, since

$$\langle X_1 | H | X_2 \rangle = \lambda_2 \langle X_1 | J | X_2 \rangle = \lambda_1^* \langle X_1 | J | X_2 \rangle .$$

For real eigenvalues this reduces to the orthogonality of the eigenvectors corresponding to different eigenvalues. In this case we have also

$$\langle X_\pm | H | X_\pm \rangle = \pm \lambda \langle X_\pm | J | X_\pm \rangle ,$$

hence one of the eigenvectors, i.e. corresponding to either $\lambda_\mu$ or $-\lambda_\mu$, has positive Krein index $\kappa$ defined as

$$\kappa(|X\rangle) = \text{sign}(\langle X | J | X \rangle) \quad (2.37)$$

since the l.h.s. is positive) and can be used as a column in the matrix $(U,V)^T$.

Thus, under the condition that the eigenvalues are semisimple, i.e. the number of the corresponding eigenvectors is equal to the algebraic multiplicity of the eigenvalue\(^3\), one can always find the first $N$ columns of the diagonalizing canonical transformation in Eq. (2.34). Then, the relation (2.36) tells us that the matrix $S$, diagonalizing $JH$ is also a canonical transformation, as in Eq. (2.34). One special case, when the eigenvalue is not semisimple, is the case of zero eigenvalue. It will be considered separately below.

Let us now verify that the canonical transformation of Eq. (2.34), i.e. satisfying the properties (2.33), indeed diagonalizes the Hamiltonian (2.31) and

\(^3\)The matrix $JH$ is not normal, unless it is block-diagonal, hence its normal Jordan form is not diagonal, in general, and there may be generalized eigenvectors – such is the case of the zero eigenvalue, see below.
compute the scalar constant $K$ which has appeared in the diagonal form (2.32). Using Eqs. (2.31), (2.25) and (2.34) we obtain

$$H = \frac{1}{2} \left( \begin{array}{c} \tilde{\mathbf{b}}^\dagger, \mathbf{b} \end{array} \right) \left( \begin{array}{cc} U^\dagger & V^\dagger \\ \tilde{V} & U \end{array} \right) \mathcal{H} \left( \begin{array}{cc} U & V^* \\ V & U^* \end{array} \right) \left( \begin{array}{c} \mathbf{b} \\ \mathbf{b}^\dagger \end{array} \right) - \frac{1}{2} \text{Tr}(A)$$

$$= \frac{1}{2} \left( \begin{array}{c} \tilde{\mathbf{b}}^\dagger, \mathbf{b} \end{array} \right) J \left( \begin{array}{cc} \Lambda & 0 \\ 0 & -\Lambda \end{array} \right) \left( \begin{array}{c} \mathbf{b} \\ \mathbf{b}^\dagger \end{array} \right) - \frac{1}{2} \text{Tr}(A)$$

$$= \tilde{\mathbf{b}}^\dagger \Lambda \mathbf{b} + \frac{1}{2} \text{Tr}(\Lambda - A).$$

Hence, using Eq. (2.34) to obtain $A = U\Lambda U^\dagger + V^*\Lambda \tilde{V}$ we have

$$K = \frac{1}{2} \text{Tr}(\Lambda - A) = \frac{1}{2} \text{Tr}( (I - U^\dagger U - \tilde{V}V^*)\Lambda ) = \frac{1}{2} \text{Tr}( (I - U^\dagger U - V^*V)\Lambda )$$

$$= -\text{Tr}(V^*V\Lambda) = -\sum \lambda_\mu \sum \nu |V_{\nu\mu}|^2. \quad (2.38)$$

The diagonalization of $J\mathcal{H}$ is intimately related to the properties of the quadratic form $\frac{1}{2}\langle X|\mathcal{H}|X \rangle$ which is a Lyapunov (energy) function for the classical Hamiltonian system $i\dot{X} = J\mathcal{H}X$, written in the complex canonical coordinates: $X = (z_1, \ldots, z_N, z_1^*, \ldots, z_N^*)$. The Hamiltonian flow is decoupled into invariant (independent) flows corresponding to the subspaces of the quartets of eigenvalues. It can be shown that the quadratic form $\langle X|\mathcal{H}|X \rangle$ has even numbers of positive and negative squares over each subspace corresponding to real eigenvalues $\text{Im}(\lambda_\mu) = 0$ (but not necessarily being definite in any of these), while it has equal number of positive and negative squares over each subspace corresponding to the eigenvalues having nonzero imaginary part, $\text{Im}(\lambda_\mu) \neq 0$. Therefore, a sufficient condition for the matrix $J\mathcal{H}$ to have real eigenvalues, i.e. the corresponding Hamiltonian flow to be stable, is the quadratic form $\langle X|\mathcal{H}|X \rangle$ be definite. This is a very crude criterion, since the quadratic form can be indefinite over the whole space, but definite in each of the invariant subspaces which property is sufficient for the matrix $J\mathcal{H}$ to have real eigenvalues only. We still have to show that the definiteness of $\mathcal{H}$ excludes the generalized eigenvectors of $J\mathcal{H}$ (we have used that the eigenvalues are semisimple). Consider a definite $\mathcal{H}$, then the matrix $B = \text{sign}(\mathcal{H})J\mathcal{H}J$ is positive. Suppose that there exists a generalized eigenvector $|X_1\rangle$ for the eigenvalue $\lambda$ and the eigenvector $|X_0\rangle$, i.e.

$$J\mathcal{H}|X_1\rangle = \lambda |X_1\rangle + |X_0\rangle, \quad J\mathcal{H}|X_0\rangle = \lambda |X_0\rangle.$$ We have then

$$J\mathcal{H}J |X_1\rangle = \lambda^2 |X_1\rangle + 2\lambda |X_0\rangle,$$

hence

$$B^\dagger J\mathcal{H}B^\dagger |\tilde{X}_1\rangle = \lambda^2 |\tilde{X}_1\rangle + |\tilde{X}_0\rangle, \quad B^\dagger J\mathcal{H}B^\dagger |\tilde{X}_0\rangle = \lambda^2 |\tilde{X}_0\rangle,$$
where
\[ | \tilde{X}_1 \rangle \equiv B^{-1} | \tilde{X}_1 \rangle, \quad | \tilde{X}_0 \rangle \equiv 2 \lambda B^{-1} | \tilde{X}_0 \rangle, \]
which is a contradiction, since the matrix \( B^\dagger H B^\dagger \) is Hermitian and cannot have generalized eigenvectors.

### 2.2.1 Diagonalization of the quadratic bosonic Hamiltonian possessing a zero mode

Let us consider now the special case, when there is a zero eigenvalue of the matrix \( J^\dagger H \) (2.34) used in the diagonalization of the quadratic bosonic Hamiltonian (2.31). Let us assume that there is just one eigenvector \( |X_0\rangle \), also called the zero mode, corresponding to the zero eigenvalue, i.e. \( J^\dagger H |X_0\rangle = 0 \). Then \( \tau |X_0\rangle^* = e^{i\theta} |X_0\rangle \), with some phase \( \theta \) (evident from \( \tau (\tau |X_0\rangle^*)^* = |X_0\rangle \)). Note that the phase \( \theta \) can be set to zero by multiplication of the zero mode by \( e^{i\pi/2} \). We have then
\[ |X_0\rangle = \begin{pmatrix} G \\ G^* \end{pmatrix}, \quad J^\dagger H |X_0\rangle = 0, \quad (2.39) \]
where \( G \) is a column. This fact disallows one to use the zero mode as one of the columns in the construction of the transformation matrix (2.34), otherwise it will not have the inverse and hence, the boson commutation relations will not be satisfied by the new operators.

However the remedy is in the eigenvalue problem itself, which is not Hermitian and allows the existence of the generalized eigenvectors. There is at least one of them. Indeed, we have for the first generalized eigenvector the following problem
\[ J^\dagger H |X_1\rangle = |X_0\rangle. \quad (2.40) \]
Due to the fact that \( \langle X_0 | H = 0 \) and \( \langle X_0 | J | X_0 \rangle = 0 \), such a generalized eigenvector \( |X_1\rangle \) exists by the Fredholm alternative. Note that Eqs. (2.39) and (2.40) give \( \tau |X_1\rangle^* = -|X_1\rangle \), i.e. the general form of the generalized eigenvector reads
\[ |X_1\rangle = \begin{pmatrix} F \\ -F^* \end{pmatrix}, \quad (2.41) \]
where \( F \) is a column.

We assume the simplest case, when there are no higher generalized eigenvectors, by assuming the condition \( \langle X_0 | J | X_1 \rangle = \langle X_1 | H | X_1 \rangle \neq 0 \) (the product is then positive), which disallows the existence of the higher eigenvector \( |X_2\rangle \), i.e. the corresponding equation
\[ J^\dagger H |X_2\rangle = |X_1\rangle \]
by the Fredholm alternative has no solutions. Below the vectors \( |X_0\rangle \) and \( |X_1\rangle \) are assumed to be normalized such that \( \langle X_0 | J | X_1 \rangle = 1 \) (since their product is
always positive, the normalization does not change the form of the eigenvectors given by Eqs. (2.39) and (2.41)). Introduce the following normalized vector

$$|Z⟩ = \begin{pmatrix} Z_U \\ Z_V \end{pmatrix} = \alpha|X_0⟩ + |X_1⟩, \quad \alpha + \alpha^* = 1,$$

(2.42)
i.e. that ⟨Z|J|Z⟩ = Z_U^T Z_U − Z_V^T Z_V = 1. Now we can construct the transformation matrix S of Eq. (2.25) having the required properties:

$$S = \begin{pmatrix} Z_U, U_⊥ \\ Z_V, V_⊥ \end{pmatrix} \equiv \begin{pmatrix} U & V^* \\ V & U^* \end{pmatrix}, \quad (2.43)$$

where the matrices U_⊥ and V_⊥ correspond to the non-zero eigenvalues of JH. Due to the orthogonality of the eigenvectors corresponding to distinct eigenvalues and the normalization of |Z⟩ we have S^−1 = JS^1J as it should be. On the other hand, by construction we have τSτ = S*. The eigenvector decomposition of the transformation matrices S and S^−1 reads:

$$S = ⟨Z|, |X_μ⟩, ..., τ|Z⟩|^*, ..., τ|X_μ⟩^*, ..., ⟩, \quad S^−1 = \begin{pmatrix} ⟨Z|J \\ ⟨X_μ|J \\ ... \\ −⟨Z|^*τJ \\ −⟨X_μ|^*τJ \\ ... \end{pmatrix}, \quad (2.44)$$

where we have used the property S^−1 = JS^1J and the diagonal structure of J, which lead to the minus sign at ⟨X_μ|^*τJ. Observe that the minus sign in the inverse transformation matrix is at the vectors having negative Krein index (2.37), due to our selection as the vectors |X_μ⟩ those which have positive Krein index (since we had to satisfy the condition U^†U = V^†V = J). From Eq. (2.44) and the general theory of Jordan normal form of a matrix (using that ⟨X_0|J|X_1⟩ = 1 for vectors of the zero eigenvalue subspace), one easily derives the representation (note the appearance of the Krein index in the formula below)

$$JH = \sum_\lambda \lambda |X_\lambda⟩⟨X_\lambda|J \quad + \quad |X_0⟩⟨X_0|J \quad = \quad \sum_\lambda \lambda \kappa(|X_\lambda⟩) |X_\lambda⟩⟨X_\lambda|J + |X_0⟩⟨X_0|J$$

$$= S \begin{pmatrix} \Lambda & 0 \\ 0 & -\Lambda \end{pmatrix} S^* + |X_0⟩⟨X_0|J, \quad (2.45)$$

where Λ = diag(0, λ_2, ..., λ_N), λ_μ ≠ 0 for μ ≠ 1, |X_λ⟩ is the eigenvector corresponding to λ and the addition on the r.h.s. is the nilpotent matrix N_0, such that N_0|X_0⟩ = 0 and N_0|X_1⟩ = |X_0⟩, i.e. giving the Jordan block corresponding to the zero eigenvalue (of multiplicity 2 in our case). From Eq. (2.45) the
structure of the Hessian matrix associated with the Hamiltonian (2.31) appearing under the canonical transformation (2.43) can be calculated. First of all, using the orthogonality properties of the eigenvectors corresponding to different eigenvalues and that \( \langle Z|J|X_0 \rangle = 1 \) and \( \langle Z^\tau J|X_0 \rangle = -1 \) one can obtain the identity
\[
\langle X_0|JS(\tilde{b}^\dagger,\tilde{b}) \rangle = (1,0,\ldots,0,-1,0,\ldots,0) \begin{pmatrix} b \\ b^\dagger \end{pmatrix} = b_1 - b_1^\dagger. \tag{2.46}
\]
Using this identity and Eqs. (2.39)–(2.45) we get
\[
H = \frac{1}{2} \left( \begin{pmatrix} \Lambda & 0 \\ 0 & \Lambda \end{pmatrix} + S^\dagger J|X_0\rangle\langle X_0|JS \right) \begin{pmatrix} b \\ b^\dagger \end{pmatrix} - \frac{1}{2} \text{Tr}(A)
\]
\[
= \frac{1}{2} \left( \begin{pmatrix} b^\dagger_1 - b_1 \\ b_1 - b^\dagger_1 \end{pmatrix} \right) + \text{Tr}(\Lambda - A) \tag{2.47}
\]
Note the appearance of the non-diagonalized part expressed through the new operators \( b_1 \) and \( b^\dagger_1 \). It is easy to see that this addition represents the simplest one-mode bosonic Hamiltonian quadratic in the boson operators,
\[
H_1 \equiv \frac{1}{2} (b^\dagger_1 - b_1)(b_1 - b^\dagger_1) = \frac{1}{2} \left( b^\dagger_1 b_1 + b_1 b^\dagger_1 - b^2_1 - (b^\dagger_1)^2 \right),
\]
which cannot be diagonalized. Indeed, let us perform the canonical change of variables to the real observables \( Q \) and \( P \), defined as follows
\[
Q_1 \equiv \frac{b_1 + b^\dagger_1}{\sqrt{2}}, \quad P_1 \equiv \frac{b_1 - b^\dagger_1}{i\sqrt{2}}, \quad [P_1, Q_1] = -i. \tag{2.48}
\]
Then \( H_1 = P_1^2 \) which has a continuous spectrum as distinct from a one-mode quadratic Hamiltonian which is diagonalizable to the standard form \( \sim c^\dagger c \). This continuous spectrum is a consequence of the symmetry breaking in the associated classical Hamiltonian system with the same Hessian \( \mathcal{H} \), a feature which leads to the existence of the zero modes. Therefore, in the quantum case, the classical symmetry breaking leads to the appearance of degrees of freedom with a continuous spectrum. Now, we can write the Hamiltonian (2.47) in its final form
\[
H = P_1^2 + \sum_{\lambda_\mu \neq 0} \lambda_\mu b^\dagger_\mu b_\mu + \frac{1}{2} \left[ \sum_\mu \lambda_\mu - \text{Tr}(A) \right]. \tag{2.49}
\]
Finally, let us express the canonical observables \( P_1 \) and \( Q_1 \) through the old bosonic operators \( a_\mu \) and \( a^\dagger_\mu \). From Eq. (2.46) and the canonical transformation (2.25) we get
\[
P_1 = \frac{i}{\sqrt{2}} \langle X_0|J(\begin{pmatrix} a \\ a^\dagger \end{pmatrix}) = \frac{i}{\sqrt{2}} \sum_\mu \left( G_\mu a^\dagger_\mu - G^*_\mu a_\mu \right). \tag{2.50}
\]
On the other hand, Eqs. (2.39), (2.41), (2.42) and (2.44) give

\[ b_1 = \langle Z | J \left( \begin{array}{c} a \\ a^\dagger \end{array} \right) = \sum_\mu \left[ (Z_\mu^0) a_\mu - (Z_\mu^V) a^\dagger_\mu \right] \]

\[ = \sum_\mu \left\{ \left[ \alpha^* G_\mu + F_\mu^* \right] a_\mu + [F_\mu - \alpha^* G_\mu] a^\dagger_\mu \right\}. \]  

(2.51)

Therefore, by the definition (2.48) and that \( \alpha + \alpha^* = 1 \) we obtain

\[ Q_1 = \sqrt{2} \sum_\mu (F_\mu a_\mu^\dagger + F_\mu^* a_\mu) + 2 \text{Im}(\alpha) P_1 = \sqrt{2} \langle X_1 | J \left( \begin{array}{c} a \\ a^\dagger \end{array} \right) \rangle + 2 \text{Im}(\alpha) P_1. \]  

(2.52)

The zero mode \(|X_0\rangle\) and the generalized eigenvector \(|X_1\rangle\) define the respective canonical operators. Observe that there is some arbitrariness in the definition of \( Q_1 \) related to the arbitrariness in the choice of \( \alpha \) in Eq. (2.42). One can verify the commutation relations (2.48) are satisfied using that

\[ 2 \sum_\mu F_\mu^* G_\mu = \langle X_0 | J | X_1 \rangle = 1. \]

2.3 Long range order, condensation and the Bogoliubov spectrum of weakly interacting Bose gas

Consider an interacting Bose gas trapped in an external potential \( V(|r|) \) and interacting with the two-body potential \( U(|r|) \). The Hamiltonian of the system in the second quantization representation reads (see Eq. (1.68))

\[ H = \int d^3r \left\{ \psi^\dagger(r) \left( \frac{-\hbar^2}{2m} \nabla^2 \right) \psi(r) + V(r) \psi^\dagger(r) \psi(r) \right\} 
\]

\[ + \frac{1}{2} \int d^3r \int d^3r' U(|r - r'|) \psi^\dagger(r) \psi^\dagger(r') \psi(r') \psi(r). \]  

(2.53)

According to the Penrose & Onsager criterium [2], there is a condensation in the system of bosons, related also to the concept of the long range order (see also Ref. [3]), if the one-particle statistical operator \( \sigma_1 \), defined in Eq. (1.89), has an eigenvalue on the order of the total number of particles (we will use \( \sigma_1 \) instead of \( R_1 \) since the approach is applicable for the variable total number of particles and in our case it is not fixed). Let us denote by \(|\Phi_0\rangle\) the eigenstate of \( \sigma_1 \) with the macroscopic eigenvalue \( \langle n_0 \rangle \sim \langle N \rangle \). It is a state from the single-particle Hilbert space (the eigenvalue \( \langle n_0 \rangle \) is the average population of this state, see also Eq. (1.91) of section 1.7.2). One could expand the operator \( \sigma_1 \) in the basis of its eigenstates, however, below we will see that one must choose another basis for the expansion in the complement of the Hilbert space orthogonal to the macroscopically occupied state \(|\Phi_0\rangle\). For now we assume that the basis states
\( |\Phi_\alpha\rangle \), \( \alpha \geq 0 \) are taken from the single-particle Hilbert space. The statistical operator \( \sigma_1 \) assumes the following form (we assume that the basis is countable and the eigenfunctions are integrable in the coordinate representation)

\[
\sigma_1 = \langle a^\dagger_\alpha a_\alpha | \Phi_0 \rangle |\Phi_0\rangle + \sum_{\alpha, \beta \geq 1} \langle a^\dagger_\alpha a_\beta | \Phi_\beta \rangle |\Phi_\beta\rangle \equiv \langle a^\dagger_0 a_0 | \Phi_0 \rangle |\Phi_0\rangle + \sigma_1^{(\perp)}.
\] (2.54)

The coefficients of this expansion are easily found by the observation that (see Eq. (1.90) of section 1.7.1)

\[
\langle \Phi_\beta | \sigma_1 | \Phi_\alpha \rangle = \langle a^\dagger_\alpha a_\beta \rangle,
\]

where the boson operator \( a_\alpha \) annihilates the state \( |\Phi_\alpha\rangle \), i.e. it appears in the expansion of the annihilation operator \( \Psi(r) \):

\[
\Psi(r) = \sum_\alpha \Phi_\alpha(r) a_\alpha.
\] (2.55)

The assumption of the long range order, i.e. \( \langle n_0 \rangle = \langle a^\dagger_0 a_0 \rangle \sim \langle N \rangle \), is complemented that there is just one macroscopically occupied state, i.e. the eigenvalues \( n_1^{(\perp)} \) of the orthogonal complement \( \sigma_1^{(\perp)} \) satisfy \( n_1^{(\perp)} \ll \langle n_0 \rangle \). Then, for instance, the occupations of the states \( \Phi_\alpha, \alpha \geq 1 \), are also small \( \langle a^\dagger_\alpha a_\alpha \rangle \ll \langle N \rangle \). The trace of \( \sigma_1 \) is equal to the average of the total number of atoms, i.e. we have \( \sum_\alpha \langle a^\dagger_\alpha a_\alpha \rangle = \langle N \rangle \).

Following C.N. Yang [3], one can easily show that in this case any statistical operator \( \sigma_s \) of the system of bosons has an eigenvalue \( \sim \langle N \rangle \), for instance \( \sigma_2 \) has the largest eigenvalue which is bound as follows \( \langle n_0 \rangle (\langle n_0 \rangle - 1) \leq \sigma_2 \leq \langle N (N - 1) \rangle \). This is clear from the following calculation \( \langle a^\dagger_0 a_0 a_0 a_0 \rangle = \langle n_0^2 \rangle - \langle n_0 \rangle \geq \langle n_0 \rangle^2 - \langle n_0 \rangle \), whereas the latter term is one of the diagonal terms of \( \sigma_2 \) in the above used basis and is clearly less than the maximal eigenvalue of \( \sigma_2 \). The statistical operators \( \sigma_{1,2} \) are those used in the calculation of the average energy of the system, thus the long range order allows to approximate the expression for the system energy in the orders of \( \langle n_0 \rangle \) (see below).

In the basis (2.55) the Hamiltonian reads

\[
H = \sum_{\alpha, \beta} E_{\alpha, \beta} a^\dagger_\alpha a_\beta + \frac{1}{2} \sum_{\alpha_1, \alpha_2, \beta_1, \beta_2} U_{\alpha_1, \alpha_2, \beta_1, \beta_2} a^\dagger_{\alpha_1} a_{\alpha_2} a_{\beta_1} a^\dagger_{\beta_2},
\] (2.56)

where the single-particle part of the Hamiltonian and the interaction part have the following expansion coefficients:

\[
E_{\alpha, \beta} = \int d^3r \left\{ \Phi^*_\alpha(r) \left( -\frac{\hbar^2}{2m} \nabla^2 \right) \Phi_\beta(r) + \Phi^*_\alpha(r) V(r) \Phi_\beta(r) \right\}
\] (2.57)

\[
U_{\alpha_1, \alpha_2, \beta_1, \beta_2} = \int d^3r \int d^3r' U(|r - r'|) \Phi^*_\alpha_1(r) \Phi^*_\alpha_2(r') \Phi_{\beta_1}(r') \Phi_{\beta_2}(r).
\] (2.58)
In the following we will use the evident properties of these coefficients:

\[ E_{\alpha,\beta} = (E_{\beta,\alpha})^*, \quad U_{\beta_1,\beta_2}^{\alpha_1,\alpha_2} = (U_{\alpha_1,\alpha_2}^{\beta_1,\beta_2})^*, \quad U_{\beta_1,\beta_2}^{\alpha_1,\alpha_2} = U_{\beta_2,\beta_1}^{\alpha_2,\alpha_1}. \]  

(2.59)

The long range order assumption allows us to use the successive approximations of the system Hamiltonian (2.56) in the perturbation theory with the small parameter \( \langle n_0 \rangle^{-1/2} \). This assumption is sometimes related to the appearance of a macroscopic order parameter and is related to the classical limit of quantum description. However, one should yet supplement the long range order condition by an additional one before one could talk about a macroscopic order parameter. Namely, that the distribution of the occupation number \( n_0 = a_0^\dagger a_0 \) is peaked at the average value, i.e.

\[ \sqrt{\langle (n_0 - \langle n_0 \rangle)^2 \rangle} \ll \langle n_0 \rangle. \]  

(2.60)

We will also assume the practically relevant condition that the mean-field potential created by the interaction between the bosons, i.e. the average interaction potential, has the same order as the kinetic term:

\[ U_{0,0}^{0,0} \sim E_{0,0}. \]  

(2.61)

Under this assumption, one can approximate the average value of the Hamiltonian in Eq. (2.56) in the leading order in \( \langle n_0 \rangle \) as follows

\[ \langle H \rangle = E_{0,0}(n_0) + \frac{U_{0,0}^{0,0}}{2} (n_0(n_0-1)) + \mathcal{O}(\sqrt{\langle n_0 \rangle}) \approx E_{0,0}(n_0) + \frac{U_{0,0}^{0,0}}{2} \langle n_0 \rangle^2 + \mathcal{O}(\sqrt{\langle n_0 \rangle}) \]

\[ \equiv \langle H^{(0)} \rangle + \mathcal{O}(\sqrt{\langle n_0 \rangle}). \]  

(2.62)

We have denoted by \( H^{(0)} \) the leading term of the Hamiltonian on the order \( \mathcal{O}(\langle n_0 \rangle) \). It can be put in the form of the so-called Gross-Pitaevskii functional, i.e.

\[ \langle H^{(0)} \rangle = E_{GP}(\Psi_0^*, \Psi_0) = \int d^3r \left\{ \Psi_0^*(r) \left( -\frac{\hbar^2}{2m} \nabla^2 \right) \Psi_0 + V(r)|\Psi_0(r)|^2 \right\} \]

\[ + \frac{1}{2} \int d^3r \int d^3r' U(|r - r'|)|\Psi_0(r)|^2|\Psi_0(r')|^2, \]  

(2.63)

by introducing the order parameter \( \Psi_0(r) = \langle n_0 \rangle \Phi_0(r) \) of the condensate [6].

To find the equation defining the order parameter, consider the ground state of the system, which is the extremal of the average energy

\[ \overline{E}(\langle G \rangle, \langle G \rangle) \equiv \frac{\langle G | H | G \rangle}{\langle G | G \rangle}, \]  

(2.64)

---

4 Here and below, the order of the approximations to the Hamiltonian, the chemical potential and the free energy are denoted by the superscript in brackets. These correspond to the orders of correction these quantities describe in the perturbation theory and do not correspond to respective powers of \( \langle n_0 \rangle \) the approximations give.
where $|G\rangle$ is the tentative system state. Indeed, variation of $E(|G\rangle, \langle G|)$ with respect to the bra-vector $\langle G|$ leads to the Euler-Lagrange equation $H|G\rangle = E(|G\rangle, \langle G||G\rangle)$. In our case it should be taken under the condition that the average number of bosons $\langle N \rangle$ is fixed. To account for the latter condition, one can use the functional

$$F(|G\rangle, \langle G|) = E(|G\rangle, \langle G|) - \mu \frac{\langle G|N|G\rangle}{\langle G||G\rangle}$$

(2.65)

with the Lagrange multiplier $\mu$. The purpose of the functional $F$ is to convert the constrained minimization problem into an unconstrained one, the $\mu$ is defined by equating the derivative over $\langle N \rangle$ to zero: $\frac{\partial F}{\partial \langle N \rangle} = 0$, thus we have $\mu = \frac{\partial E}{\partial \langle N \rangle}$.

The order parameter or the “condensate wave function” $\Psi_0(r)$ can be found by minimizing the functional $F$ (2.65), which in the made approximation ($N \approx n_0$) becomes

$$F_{GP} = E_{GP}(\Psi_0^*, \Psi_0) - \mu^{(0)} \int d^3r |\Psi_0(r)|^2,$$

(2.66)

where that the Lagrange multiplier $\mu^{(0)}$ now accounts for the normalization of the order parameter: $\int d^3r |\Psi_0(r)|^2 = \langle n_0 \rangle$. Taking the first variation in $\Psi_0^*(r)$ and setting $\Psi_0(r) = \langle n_0 \rangle \Phi_0(r)$ we obtain the Euler-Lagrange equation for the strongly occupied state

$$\mu^{(0)} \Phi_0(r) = -\frac{\hbar^2}{2m} \nabla^2 \Phi_0(r) + \langle n_0 \rangle \left\{ \int d^3r' U(|r - r'|) |\Phi_0(r')|^2 \right\} \Phi_0(r).$$

(2.67)

Multiplying this equation by $\Phi^*(r)$ and integrating we obtain the chemical potential

$$\mu^{(0)} = \mathcal{E}_{0,0} + \langle n_0 \rangle U_{0,0}^{0,0}.$$

(2.68)

The next order approximation to the energy of a gas in an external potential will be considered below after we consider a much simpler system – the weakly interacting Bose gas in a box, whose excitation spectrum was considered by N.N. Bogoliubov [4].

### 2.3.1 The excitation spectrum of weakly interacting Bose gas in a box

Consider the weakly interacting Bose gas in free space. We will work in a three dimensional box $V = L^3$ of the size $L$, and consider the limit $L \to \infty$. By weakly we mean that the average potential created due to the interaction between the bosons is negligible compared to the kinetic energy of the bosons. Then the strongly occupied state in this case is the zero-momentum state $p = 0$ (which is approximately the ground state of the system in our case). Thus we will use the momentum states for the expansion, i.e. $\Phi_\alpha(r) = \frac{1}{\sqrt{V}} e^{i p_\alpha r / \hbar}$, where $p_\alpha = \frac{2\pi n_\alpha}{L}$ with $n_\alpha$ being three dimensional vector taking integer values. The
Hamiltonian (2.53) in this case has the following form (we use the summation over the discrete momenta $p$)

$$H = \sum_p \frac{p^2}{2m} a_p^\dagger a_p + \frac{1}{2} \sum_{p_1, p_2 \neq p_1, p_2} \frac{\hat{U}(p_1 - p_2)}{V} \delta_{p_1 + p_2, p_1'} \delta_{p_2 + p_1', p_2'} a_{p_1'}^\dagger a_{p_2'} a_{p_1} a_{p_2},$$  \hspace{1cm} (2.69)

where $\hat{U}$ is the Fourier transform of the interaction potential,

$$\hat{U}(p) = \int d^3 r \ e^{i \frac{p}{\hbar} r} \bar{U}(\frac{\hbar}{|r|}) = 4\pi \bar{\hbar} \int d^3 r \ r^2 U(r) \sin \left( \frac{p}{\bar{\hbar}} r \right),$$  \hspace{1cm} (2.70)

which is obviously a function of $p^2 = p^2$. For the diagonalization of the quadratic form (the form $F^{(2)}$ (2.77) below) to be possible one must demand that for all $p \neq 0$ the Fourier transform of the interaction is non-negative $\hat{U}(p) \geq 0$. This condition is satisfied, for instance, by the zero-range repulsive interactions $U(r) = g\delta(r)$ with $g > 0$.

The leading order part of the Hamiltonian (2.69) is

$$H^{(0)} = \frac{1}{2} \frac{\hat{U}(0)}{V} n_0 (n_0 - 1),$$

thus using the unconstrained minimization problem for $\langle F(0) \rangle = \langle H^{(0)} \rangle - \mu^{(0)} n_0$ and the assumption (2.60) we get approximately $\mu^{(0)} = \frac{\hat{U}(0)}{V}(n_0)$. Taking into account the momentum conservation (given by the delta-symbol in Eq. (2.69)) we get the next order of $H$ as follows (note that this term is actually a fourth order term in the boson operators and preserves the total number of bosons in the system)

$$H^{(2)} = \sum_{p \neq 0} \left[ \frac{p^2}{2m} + \left( \frac{\hat{U}(0)}{V} + \frac{\hat{U}(p)}{V} \right) n_0 \right] a_p^\dagger a_p^\dagger$$

$$+ \frac{1}{2} \frac{\hat{U}(p)}{V} \left\{ (a_0^\dagger)^2 a_{-p} a_{-p} + (a_0)^2 a_p a_p^\dagger \right\}.$$  \hspace{1cm} (2.72)

Below, we work with the free energy operator $F = H - \mu N$ instead of the Hamiltonian. We also note that, due to the momentum conservation and weak interaction, the expansion of the free energy contains no first order term, i.e.

$$F = F^{(0)} + F^{(2)} + \ldots = H^{(0)} - \mu^{(0)} n_0 + H^{(2)} - \mu^{(2)} N^{(2)} - \mu^{(2)} n_0 + \ldots,$$

where $N^{(2)} = \sum_{p \neq 0} a_p^\dagger a_p$.

In the next order approximation to the Hamiltonian (more precisely, to the average energy functional (2.64)) is given by the terms quadratic in the creation and annihilation operators $a_p^\dagger$ and $a_p$ for $p \neq 0$ due to the momentum conservation by the interaction term. To see how the averages involving $a_0^\dagger$ or $a_0$ can
be approximated in our approach we introduce the polar decomposition of the operators $a_0^\dagger$ and $a_0$:

$$
a_0^\dagger = e^{i\phi_0} \sqrt{n_0 + 1} = \sqrt{n_0} e^{i\phi_0}, \quad a_0 = e^{-i\phi_0} \sqrt{n_0} = \sqrt{n_0 + 1} e^{-i\phi_0},
$$

(2.73)

where the shift operator $e^{i\phi_0}$ acts in the following way on the Fock state

$$
e^{i\phi_0} |n_0 \rangle = |n_0 + 1 \rangle.
$$

(2.74)

The following immediate identities are found by application of Eq. (2.73)

$$
e^{-i\phi_0} e^{i\phi_0} = I - |N_0 \rangle \langle N_0|, \quad e^{i\phi_0} e^{-i\phi_0} = I - |0 \rangle \langle 0|,
$$

(2.75)

where $|N_0 \rangle$ is the state with the maximal occupation number, if it exists. Thus, strictly speaking, the shift operator is not unitary (hence, the “phase” $\phi_0$ is not Hermitian operator). However, in our case we can safely approximate $e^{i\phi_0} e^{-i\phi_0} = e^{-i\phi_0} e^{-i\phi_0} = I$ neglecting the states of $n_0 = 0$ and $n_0 = N_0$ (the latter state corresponds to all atoms occupying the state $\Phi_0(r)$) which are the boundary states and are not important. In this approximation, we can perform the transformation

$$
\hat{a}_p = e^{i\phi_0} a_p, \quad \hat{a}_p^\dagger = e^{-i\phi_0} a_p^\dagger, \quad p \neq 0,
$$

(2.76)

which is obviously canonical one (note that the shift operator commutes with the orthogonal degrees of freedom described by the operators $a_p$ with $p \neq 0$).

In this respect we should mention the recent results on the validity of the $U(1)$-symmetry breaking approach, where it is argued that one can substitute the operators $a_0$ and $a_0^\dagger$ by the classical variables in the Hamiltonian augmented by a symmetry-breaking term [7].

Using the canonical transformation (2.76), the identities $a_0^2 = e^{-2i\phi_0} \sqrt{n_0(n_0 - 1)}$ and (2.75), replacing the operator $n_0$ by its average value due to the assumption (2.60), we get the second order correction to the free energy $F$, i.e. $F^{(2)} = H^{(2)} - \mu^{(0)} N^{(2)}$ (where the scalar term $-\mu^{(2)} \langle n_0 \rangle$ is inessential and dropped), as follows

$$
F^{(2)} = \sum_{p \neq 0} \left\{ \frac{p^2} {2m} + \frac{\hat{U}(p)} {V} \langle n_0 \rangle \right\} \hat{a}_p^\dagger \hat{a}_p + \frac{1} {2} \frac{\hat{U}(p)} {V} \left[ \langle n_0 \rangle^2 \hat{a}_p^\dagger \hat{a}_p + \langle n_0 \rangle^2 \hat{a}_p \hat{a}_p^\dagger - p^2 \right].
$$

(2.77)

Note that $F^{(2)}$ consists of block operators for each value of $p$. Each such block can be diagonalized by the Bogoliubov transformation which involves just two modes with the opposite momenta: $p$ and $-p$. Denoting

$$
\alpha(p^2) = \frac{p^2} {2m} + \frac{\hat{U}(p)} {V} \langle n_0 \rangle, \quad \beta(p^2) = \frac{\hat{U}(p)} {V} \langle n_0 \rangle^2
$$

(2.78)

we can write $F^{(2)} = \sum_p f_p^{(2)}$ where each $p$-block is in the standard form (note that we use two term block: the term with $p$ and with $-p$ enter each block,
hence the free term is twice the free term for $p$

\[ F_p^{(2)} = \frac{1}{2} (a_p^\dagger, a_{-p}^\dagger, a_p, a_{-p}) \begin{pmatrix} A_p & B_p \\ B_p & A_p \end{pmatrix} \begin{pmatrix} a_p \\ a_{-p}^\dagger \\ a_{-p}^\dagger \\ a_p \end{pmatrix} - \alpha(p^2), \quad (2.79) \]

where

\[ A_p = \begin{pmatrix} \alpha(p^2) & 0 \\ 0 & \alpha(p^2) \end{pmatrix}, \quad B_p = \begin{pmatrix} 0 & \beta(p^2) \\ \beta(p^2) & 0 \end{pmatrix}, \]

note that both $A_p$ and $B_p$ are real. According to the general theory of section 2.2 the diagonalization of the quadratic form given in Eq. (2.79) is performed by the transformation composed of the eigenvectors of the matrix $JH$ with the Hessian defined in Eq. (2.79) by the matrices $A_p$ and $B_p$. We obtain the characteristic polynomial $\chi(\lambda) = \det(JH - \lambda I)$ in the form $\chi(\lambda) = (\lambda^2 + \beta^2 - \alpha^2)^2$ thus the eigenvalues $\lambda_{\pm} = \pm \sqrt{\alpha^2 - \beta^2}$ are doubly degenerate. The eigenvectors $|\lambda\rangle$ can be easily found, the right normalization eigenvectors, i.e. satisfying $\langle \lambda | J | \lambda \rangle = 1$ correspond to the positive eigenvalues $\lambda_+$. We have the transformation matrix $S$ in the form

\[ S = \begin{pmatrix} U & V \\ V & U \end{pmatrix} \]

(2.80)

where

\[ U = \frac{1}{\sqrt{2(\alpha^2 - \beta^2)^2}} \begin{pmatrix} \sqrt{\alpha^2 - \beta^2} & \beta \\ 0 & \beta \end{pmatrix}, \quad V = \frac{1}{\sqrt{2(\alpha^2 - \beta^2)^2}} \begin{pmatrix} \beta & \sqrt{\alpha^2 - \beta^2} \\ 0 & \sqrt{\alpha^2 - \beta^2} \end{pmatrix}. \]

For instance, we obtain the excitation spectrum, the Bogoliubov spectrum as follows

\[ E(p^2) = \lambda_+ = \sqrt{\alpha^2 - \beta^2} = \sqrt{\frac{p^2}{2m} \left( \frac{p^2}{2m} + \frac{2\hat{U}(p)}{V} \langle n_0 \rangle^2 \right) }. \quad (2.81) \]

The Bogoliubov transformation (2.25) makes the operator $F^{(2)}$ diagonal

\[ F^{(2)} = \sum_{p \neq 0} E(p^2) \hat{b}^\dagger_p \hat{b}_p - \sum_{p^2} (E(p^2) - \alpha(p^2)). \quad (2.82) \]

### 2.3.2 The excitation spectrum of an interacting Bose gas in an external potential

Let us now return to the general case of a Bose gas in an external potential, which we have started to consider in section 2.3. The interaction is not assumed
to be negligible as for the gas in a box considered above, but on the order of the single-particle energy term, as in Eq. (2.61). We will consider the next two terms of the approximation in the orders of $\langle n_0 \rangle$ of the Hamiltonian (2.56). First of all, similar as in the case of the gas in a box, the condition of the long range order, supplemented by the conditions (2.60) and (2.61), allows us to separate the amplitude and phase of the creation and annihilation operators $a_0 = e^{-i\varphi_0}\sqrt{n_0}$ and $a_0^\dagger = \sqrt{n_0}e^{i\varphi_0}$, as in Eq. (2.73). Thus, similar as in the case of a gas in a box, Eq. (2.76), we perform a canonical transformation on the rest of the boson operators, corresponding to the orthogonal modes:

$$\hat{a}_\alpha = e^{i\varphi_0}a_\alpha, \quad \hat{a}_\alpha^\dagger = e^{-i\varphi_0}a_\alpha^\dagger, \quad \alpha \geq 1.$$ (2.83)

The next order approximation to the Hamiltonian (2.56), which follows $\mathcal{E}$ (2.63) in the expansion in the orders of $\langle n_0 \rangle$, is linear in the creation and annihilation operators $a_\alpha^\dagger$ and $a_\alpha$, for $\alpha \geq 1$:

$$H^{(1)} = \sum_{\alpha \geq 1} \left\{ \mathcal{E}_{\alpha,0}a_0 + U_{\alpha,0,\alpha,0}a_0^\dagger a_\alpha^\dagger + \mathcal{E}_{0,\alpha}a_\alpha^\dagger + U_{0,0,\alpha,0}(a_\alpha^\dagger a_\alpha) a_0 \right\}$$

$$= \sum_{\alpha \geq 1} \left\{ C_\alpha \hat{a}_\alpha^\dagger + C_\alpha^* \hat{a}_\alpha \right\},$$ (2.84)

where we have defined the coefficients

$$C_\alpha = \left[ \mathcal{E}_{\alpha,0} + U_{\alpha,0,\alpha,0} \right] \sqrt{n_0}$$ (2.85)

and in the derivation used the properties (2.59). The conditions (2.60) and (2.61) allow us to replace $n_0$ in the definition of $C_\alpha$ by the scalar $\langle n_0 \rangle$ which substitution turns the coefficient into a scalar. The definition of this scalar coefficient has the form of a “matrix element” of the average boson energy in the macroscopically occupied state, i.e. the Bose-Einstein condensate, between the two single particle states $\ket{\Phi_0}$ and $\ket{\Phi_\alpha}$ for $\alpha \geq 1$ (see the definitions (2.57) and (2.58)). Here the operator $\mathcal{E}$ is the single-particle energy

$$\mathcal{E} \equiv -\frac{\hbar^2}{2m}\nabla^2 + V(r),$$ (2.86)

while the condensate energy also involves the average interaction potential defined as

$$\mathcal{U}_0(r) \equiv \langle n_0 \rangle \int d^3r' U(|r - r'|)|\Phi_0(r')|^2 = \int d^3r' U(|r - r'|)|\Psi_0(r')|^2.$$ (2.87)

But then, using the equation (2.67), which the order parameter $\ket{\Phi_0}$ satisfies, one immediately concludes that $C_\alpha = 0$:

$$C_\alpha = \sqrt{\langle n_0 \rangle}\langle \Phi_\alpha | \mathcal{E} + \mathcal{U}_0 | \Phi_0 \rangle = \mu(0) \sqrt{\langle n_0 \rangle}\langle \Phi_\alpha | \Phi_0 \rangle = 0, \quad \alpha \geq 1.$$ (2.88)

Therefore, $C_\alpha = 0$ for the arbitrary basis $\ket{\Phi_\alpha}$, $\alpha \geq 1$, from the complement of the single-particle Hilbert space orthogonal to $\ket{\Phi_0}$. Note that the corresponding
correction to the free energy $F^{(2)} = H^{(2)} - \mu^{(0)} N^{(2)} = 0$, since the term $-\mu^{(0)} N^{(1)} - \mu^{(1)} n_0$ is also identically zero ($\mu^{(1)} = \frac{\partial H^{(1)}}{\partial (n_0)} = 0$ and $N^{(1)} = 0$).

We see that the first non-zero correction after $H^{(0)}$ to the Hamiltonian (2.56), and, hence, to the free energy $F$, is quadratic in the operators $a_\alpha^\dagger$ and $a_\alpha$, $\alpha \geq 1$. We obtain this quadratic term in the following form (note that the term $F^{(2)}$ is forth order in the boson operators and *preserves* the total number of bosons in the system, as it should be)

$$F^{(2)} = H^{(2)} - \mu^{(0)} N^{(2)} = \sum_{\alpha,\beta \geq 1} \left[ \mathcal{E}_{\alpha,\beta} + \left( U_{\alpha,0}^{\alpha,0} + U_{0,\beta}^{\alpha,0} \right) n_0 - \mu^{(0)} \delta_{\alpha,\beta} \right] a_\alpha^\dagger a_\beta$$

$$+ \frac{1}{2} \sum_{\alpha,\beta \geq 1} U_{\alpha,0}^{\alpha,0} a_\alpha^\dagger a_\alpha^\dagger a_\beta^\dagger a_\beta + \frac{1}{2} \sum_{\alpha,\beta \geq 1} U_{0,\alpha}^{\alpha,0} (a_\alpha^\dagger)^2 a_\beta a_\beta,$$  \hspace{1cm} (2.89)

where $\mu^{(0)}$ is given by Eq. (2.68) and to derive this expression we have used once again the properties (2.59) (we also have used the term $\mu^{(2)} n_0$ is approximately scalar due to the assumption (2.60) and can be safely dropped). By performing the canonical transformation (2.83) in the Hamiltonian (2.89) and replacing the scalar due to the assumption (2.60), we get

$$F^{(2)} = \sum_{\alpha,\beta \geq 1} A_{\alpha,\beta} a_\alpha^\dagger a_\beta + \frac{1}{2} \sum_{\alpha,\beta \geq 1} B_{\alpha,\beta} a_\alpha^\dagger a_\beta a_\beta + \frac{1}{2} \sum_{\alpha,\beta \geq 1} B_{\alpha,\beta} a_\alpha^\dagger a_\beta,$$  \hspace{1cm} (2.90)

where we have introduced the matrices $A$ and $B$ with the matrix elements (with $\alpha \geq 1$ and $\beta \geq 1$)

$$A_{\alpha,\beta} = \mathcal{E}_{\alpha,\beta} + \left( U_{\beta,0}^{\alpha,0} + U_{0,\beta}^{\alpha,0} \right) n_0 - \mu^{(0)} \delta_{\alpha,\beta}, \hspace{1.5cm} (2.91)$$

$$B_{\alpha,\beta} = U_{0,\beta}^{\alpha,0} n_0 \hspace{1.5cm} (2.92)$$

and the obvious properties $A^\dagger = A$ and $B = B$. The quadratic form (2.90) is in the standard notations of Eq. (2.31) of section 2.2. Note the physical meaning of the interaction potential terms in the expression for $A$:

$$U_{\beta,0}^{\alpha,0} n_0 = \langle n_0 | \Phi_0^{(1)} (r') | \langle \Phi_0^{(2)} (r) | U(|r - r'|) | \Phi_0^{(1)} (r') | \Phi_0^{(2)} (r) \rangle$$

$$= \langle \Phi_0 (r) | \Phi_0 (r) \rangle \Phi_0 (r), \hspace{1.5cm} (2.93)$$

which is the matrix element of the average interaction potential created by the bosons in the condensate taken between the excitation basis states and

$$U_{0,\beta}^{\alpha,0} n_0 = \langle n_0 | \phi_0^{(1)} (r') | \langle \Phi_0^{(2)} (r) | U(|r - r'|) | \Phi_0^{(1)} (r') | \Phi_0^{(2)} (r) \rangle$$

$$= \langle \Phi_0 (r) | \Phi_0 (r) \rangle \Phi_0 (r), \hspace{1.5cm} (2.94)$$

which has the meaning of the exchange interaction between the condensed and non-condensed bosons, corresponding to the matrix element (2.93). Precisely these two terms appear in the classical linearization of the Gross-Pitaevskii energy functional about the order parameter $\Psi_0 (r)$ with the only difference
that the linearization is considered for the variations lying in the orthogonal complement to the order parameter itself. Indeed, consider the classical free energy functional (2.66) about the order parameter of the condensate, which is i.e. by Eq. (2.67) its extremal, \( \frac{\delta F_{GP}}{\delta \Psi_0(r)} = 0 \). To simplify considerably the notations, consider only the case when \( U(|r - r'|) = g\delta(r - r') \). We have the second-order correction at the order parameter \( \Psi_0(r) \) as follows

\[
F^{(2)}_{GP} = \int d^3r (\delta \Psi^\dagger(r), \delta \Psi(r)) \left[ H_{GP}(r) - \mu \right] \left( \frac{\delta \Psi(r)}{\delta \Psi^\dagger(r)} \right),
\]

where the Hessian reads

\[
H_{GP}(r) \equiv \begin{pmatrix} \mathcal{E} + 2g|\Psi_0(r)|^2 & g\Psi_0^2(r) \\ g\Psi_0^2(r) & \mathcal{E} + 2g|\Psi_0(r)|^2 \end{pmatrix},
\]

with \( \mathcal{E} \) given by Eq. (2.86). Comparing the expressions (2.95) and (2.90) with the use of the expansion (2.55) and the transformation (2.83) we observe that the quantum quadratic form \( F^{(2)} \) (2.90) can be put as follows

\[
F^{(2)} = \int d^3r (\delta \Psi^\dagger_\perp(r), \delta \Psi_\perp(r)) \left[ H_{GP}(r) - \mu \right] \left( \frac{\delta \Psi_\perp(r)}{\delta \Psi^\dagger_\perp(r)} \right),
\]

with

\[
\delta \Psi_\perp(r) \equiv \sum_{\alpha \geq 1} \hat{a}_\alpha \Phi(r).
\]

In this respect, the above approach has similarities with the approach by Y. Castin & R. Dum [8], where a systematic expansion in the fraction of the non-condensed atoms is considered without the use of the symmetry breaking. In our case, the quadratic form in \( F^{(2)} \) is also equivalent to the classical quadratic form obtained from the second-order correction to the classical free energy functional (2.66) at the order parameter if the latter is considered in the linear space of all variations orthogonal to the order parameter itself.

In our approach the zero mode corresponding to the usual \( U(1) \)-symmetry breaking in the Bogoliubov-de Gennes approach (see for instance, Ref. [9]) does not appear, since we treat the phase of the condensate as a quantum variable with an undefined value. For instance, in the extreme case, the system can be considered to be in the combination of the Fock states

\[
|G\rangle = \sum_{n_0 \ll \langle N \rangle} \sum_{\alpha \geq 1} C(\{n_\alpha\})|n_0, \{n_\alpha\}\rangle,
\]

which satisfies the long range order assumption for \( n_0 \sim \langle N \rangle \) and condition (2.60)). Instead, we use the conditions of the long range order and (2.60) which are enough to assume the classical limit, while the phase, namely, the exponential operator \( e^{i\Phi_0} \) is incorporated into the new operators \( \hat{a}_\alpha \) by a canonical transformation (2.83)).
2.4 The Jordan-Wigner transformation: fermionization of interacting 1D spin chains

In chapter 1 we have seen that the creation/annihilation operator can be defined as some linear transformation of the states of a system of indistinguishable particles which increases/decreases the total number of particles in the system and that their commutation relations can be derived. However, the commutation relations, that a set of the creation and annihilation operators satisfy, themselves define all other properties of these operators, including the structure of the associated Hilbert space, e.g. the space dimension and the Fock basis. Any system which can be described by a set of operators which satisfy the same commutation relations is thus equivalent to a system of indistinguishable particles. This is the idea of the Jordan-Wigner transformation for fermionization of the spin models.

Consider the set of operators $a_j$, $j = 1, \ldots, s$ and their Hermitian conjugates which satisfy the anti-commutation relations

$$\{a_j, a_k\} = 0, \quad \{a_j, a_k^\dagger\} = \delta_{j,k}. \quad (2.99)$$

From these it follows that $a_j^2 = 0$ and $(a_j^\dagger)^2 = 0$. Define the Hermitian operators $\hat{n}_j = a_j^\dagger a_j$. We have from Eq. (2.99)

$$\hat{n}_j^2 = a_j^\dagger a_j a_j^\dagger a_j = a_j^\dagger (-a_j^\dagger a_j + 1) a_j = a_j^\dagger a_j = \hat{n}_j, \quad (2.100)$$

$$\hat{n}_j \hat{n}_k = a_j^\dagger a_j a_k^\dagger a_k = a_j^\dagger (-a_j^\dagger a_j) a_k = a_j^\dagger a_k^\dagger a_k a_j = \ldots = \hat{n}_k \hat{n}_j, \quad k \neq j, \quad (2.101)$$

i.e. the set of the observables $\hat{n}_j$ has the common basis, where each has just two eigenvalues: 0 or 1. The eigenstates can be labelled by the occupation numbers of the operators $\hat{n}_j$ (which we will denote by $n_j$) $| n_1, n_2, \ldots, n_s \rangle$, where $n_j \in \{0, 1\}$. Moreover, from the anti-commutators (2.99) we obtain

$$[\hat{n}_j, a_k] = a_j^\dagger a_j a_k - a_k a_j^\dagger a_j = -\delta_{j,k} a_j, \quad [\hat{n}_j, a_k^\dagger] = \delta_{j,k} a_j^\dagger. \quad (2.102)$$

Hence,

$$\hat{n}_j a_j | n_1, \ldots, n_s \rangle = (n_j - 1) a_j | n_1, \ldots, n_s \rangle = 0,$$

$$\hat{n}_j a_j^\dagger | n_1, \ldots, n_s \rangle = (n_j + 1) a_j^\dagger | n_1, \ldots, n_s \rangle = a_j^\dagger | n_1, \ldots, n_s \rangle,$$

(in the first case $n_j = 1$ and in the second case $n_j = 0$, otherwise the vector itself must be zero) where the non-zero state vectors on the l.h.s. are normalized, since

$$\langle n_1, \ldots, n_s | a_j a_j^\dagger | n_1, \ldots, n_s \rangle = n_j, \quad \langle n_1, \ldots, n_s | a_j^\dagger a_j | n_1, \ldots, n_s \rangle = n_j + 1.$$

Therefore, the action of the operators $a_j^\dagger$ and $a_j$ is similar to the action of the fermionic creation and annihilation operators on the Fock states:

$$a_j | n_1, \ldots, n_j, \ldots, n_s \rangle = e^{i\varphi_j}(-) | n_1, \ldots, n_j - 1, \ldots, n_s \rangle, \quad (2.103)$$

54
where the phases \( \varphi_j^{(\pm)} \) depend on the ordering of the occupation numbers of the Fock basis states. Denoting the state \( |0, \ldots, 0\rangle \equiv |Vac\rangle \) we can set, for instance,

\[
a_j^\dagger | n_1, \ldots, n_j, \ldots, n_s \rangle = e^{i\varphi_j^{(+)} } | n_1, \ldots, n_j + 1, \ldots, n_s \rangle, \tag{2.104}
\]

then due to the anti-commutation relations (2.99) Eqs. (2.103) and (2.104) become

\[
a_j^\dagger | n_1, \ldots, n_j, \ldots, n_s \rangle = (-1)^{\sum_{k=1}^{j-1} n_k} | n_1, \ldots, n_j + 1, \ldots, n_s \rangle, \tag{2.106}
\]

\[
a_j | n_1, \ldots, n_j, \ldots, n_s \rangle = (-1)^{\sum_{k=1}^{j-1} n_k} | n_1, \ldots, n_j - 1, \ldots, n_s \rangle, \tag{2.107}
\]

where in Eq. (2.106) \( n_j = 0 \) and in Eq. (2.107) \( n_j = 1 \), otherwise the r.h.s. is zero. Indeed, we have

\[
a_j^\dagger | n_1, \ldots, n_j, \ldots, n_s \rangle = a_j^\dagger (a_j^+)^{n_1} \cdots (a_s^+)^{n_s} | Vac\rangle
\]

\[
= (-1)^{\sum_{k=1}^{j-1} n_k} (a_j^+)^{n_1} \cdots (a_j^+)^{n_j+1} \cdots (a_s^+)^{n_s} | Vac\rangle
\]

\[
= \delta_{n_j,0} (-1)^{\sum_{k=1}^{j-1} n_k} | n_1, \ldots, n_j + 1, \ldots, n_s \rangle,
\]

\[
a_j | n_1, \ldots, n_j, \ldots, n_s \rangle = a_j (a_j^+)^{n_1} \cdots (a_j^+)^{n_j} \cdots (a_s^+)^{n_s} | Vac\rangle,
\]

\[
= (-1)^{\sum_{k=1}^{j-1} n_k} (a_j^+)^{n_1} \cdots (a_j^+)^{n_j} \cdots (a_s^+)^{n_s} a_j | Vac\rangle
\]

\[
+ \delta_{n_j,1} (-1)^{\sum_{k=1}^{j-1} n_k} | n_1, \ldots, n_j - 1, \ldots, n_s \rangle
\]

\[
= \delta_{n_j,1} (-1)^{\sum_{k=1}^{j-1} n_k} | n_1, \ldots, n_j - 1, \ldots, n_s \rangle.
\]

The Hilbert space \( \mathcal{H} \) can in fact have several different vacuum states \( |Vac, \mu\rangle \) which may depend on additional observables \( \mu \). For each fixed set of observables \( \mu \) there is the Fock basis constructed above. Thus, in general, the Hilbert space can be represented as a tensor product of the Fock space and an independent space pertaining to the observables \( \mu \).

Consider now a single spin \( \frac{1}{2} \). We have the Pauli matrices

\[
\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{2.108}
\]

The eigenstates of the \( \sigma_z \) are \( |z\uparrow\rangle \) and \( |z\downarrow\rangle \) with the eigenvalues \( \pm 1 \). Denote the raising and lowering matrices \( \sigma_{\pm} \), where

\[
\sigma_+ = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} = \frac{\sigma_x + i\sigma_y}{2}, \quad \sigma_- = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} = \frac{\sigma_x - i\sigma_y}{2}, \tag{2.109}
\]

so that \( \sigma_+ |z\uparrow\rangle = 0, \sigma_+ |z\downarrow\rangle = |z\uparrow\rangle, \sigma_- |z\uparrow\rangle = |z\downarrow\rangle, \sigma_- |z\downarrow\rangle = 0 \), where \( |z\uparrow\rangle \) and \( |z\downarrow\rangle \) are spin states with a definite projection on the \( z \)-axis.
One easily observes the similarity of the operators $\sigma_\pm$ with the creation and annihilation operators, precisely we can set:

$$|0\rangle = |z \uparrow\rangle, \quad |1\rangle = |z \downarrow\rangle, \quad a = \sigma_+, \quad a^\dagger = \sigma_-.$$  \hspace{1cm} (2.110)

Then, for instance, $\sigma_z = 1 - 2\hat{n}$ by comparison of their actions on the basis states.

The above local construction, however, is invalid for the set of the spin operators $\sigma_A^{(j)}$, $j = 1, \ldots, s$, since the different spin operators commute, whereas the different fermion creation and annihilation operators satisfy the anti-commutation relations. The required correspondence between the two sets of operators must be non-local. To arrive at the required correspondence, let us recall Eqs. (2.106) and (2.107). Using that the occupation number $n_j$ corresponds to spin up $n_j = 0$ or spin down $n_j = 1$ state, that the different fermion operators $\hat{n}_j$ commute and that $1 - 2n_j = (-1)^{n_j}$ we can define the set of fermion operators for the set of the spin variables as follows

$$a_j = \left(\prod_{l=1}^{j-1} \sigma_z^{(l)}\right) \sigma_+^{(j)}, \quad a_j^\dagger = \left(\prod_{l=1}^{j-1} \sigma_z^{(l)}\right) \sigma_-^{(j)}.$$ \hspace{1cm} (2.111)

This definition is consistent with the definition of the $\sigma_z^{(j)}$ that we have started with, indeed, from Eq. (2.111) we derive

$$\sigma_z^{(j)} = \sigma_+^{(j)} \sigma_-^{(j)} - \sigma_-^{(j)} \sigma_+^{(j)} = a_j^\dagger a_j - a_j a_j^\dagger = 1 - 2\hat{n}_j.$$ \hspace{1cm} (2.112)

Thus, Eq. (2.111) can be inverted to obtain $\sigma_z^{(j)}$:

$$\sigma_+^{(j)} = \left[\prod_{l=1}^{j-1} (1 - 2\hat{n}_l)\right] a_j, \quad \sigma_-^{(j)} = \left[\prod_{l=1}^{j-1} (1 - 2\hat{n}_l)\right] a_j^\dagger.$$ \hspace{1cm} (2.113)

The other spin operators are easily derived using Eqs. (2.112) and (2.113). We have

$$\sigma_x^{(j)} = \left[\prod_{l=1}^{j-1} (1 - 2\hat{n}_l)\right] (a_j + a_j^\dagger), \quad \sigma_y^{(j)} = i \left[\prod_{l=1}^{j-1} (1 - 2\hat{n}_l)\right] (a_j^\dagger - a_j).$$ \hspace{1cm} (2.114)

In the models of interacting planar spin systems, one usually encounters the terms like the product of the neighboring spin operators, for instance, $\sigma_x^{(j)} \sigma_x^{(j+1)}$ or $\sigma_y^{(j)} \sigma_y^{(j+1)}$. These products simplify to the following expressions quadratic in the fermion operators

$$\sigma_x^{(j)} \sigma_x^{(j+1)} = (a_j^\dagger + a_{j+1})(a_j - a_{j+1}^\dagger), \quad \sigma_y^{(j)} \sigma_y^{(j+1)} = (a_{j+1}^\dagger - a_{j+1})(a_j^\dagger + a_j).$$ \hspace{1cm} (2.115)

Similar relations are valid for the cross-products of the spin components in the $xy$ plane:

$$\sigma_x^{(j)} \sigma_y^{(j+1)} = i(a_j^\dagger - a_j)(a_{j+1}^\dagger - a_{j+1}), \quad \sigma_y^{(j)} \sigma_x^{(j+1)} = i(a_{j+1}^\dagger + a_j)(a_j^\dagger + a_{j+1}).$$ \hspace{1cm} (2.116)
Therefore, any planar spin model with the next-neighbor interaction between the spins placed in the orthogonal magnetic field, i.e. describing the interacting spin components in the plane perpendicular to the magnetic field, can be mapped by the Jordan-Wigner transformation to a system of fermions described by a quadratic Hamiltonian, which then can be diagonalized by a canonical transformation of section 2.1. For example, consider the \(XY\) spin chain with the Hamiltonian

\[
H_{XY} = \sum_j \alpha_j \sigma_z^{(j)} + \sum_j \beta_j \sigma_x^{(j)} a^{(j)} a^{(j+1)} + \sum_j \gamma_j \sigma_y^{(j)} a^{(j)} a^{(j+1)},
\tag{2.117}
\]

where \(\alpha\) is proportional to the external magnetic field along the \(z\)-axis and the coefficients \(\beta\) and \(\gamma\) describe the spin interaction along the respective axes. In the fermion variables the spin Hamiltonian becomes

\[
H_{XY} = \frac{1}{2} \sum_j \left( \alpha_j (a_j^\dagger a_j - a_j a_j^\dagger) + \frac{\beta_j + i\gamma_j}{2} a_j^\dagger a_{j+1} + \frac{\beta_j - i\gamma_j}{2} a_j a_{j+1}^\dagger \right) + \frac{1}{2} \sum_j \frac{\beta_j + i\gamma_j}{2} a_j^\dagger a_j + \frac{1}{2} \sum_j \frac{\beta_j - i\gamma_j}{2} a_{j+1} a_j^\dagger. \tag{2.118}
\]


Bibliography

[1] N.N. Bogoliubov, N.N. Bogoliubov Jr., *Introduction to Quantum Statistical Mechanics* (World Scientific, Singapore, 1982).

[2] O. Penrose and L. Onsager, Phys. Rev. 104, 576 (1956).

[3] C. N. Yang, Rev. Mod. Phys. 34, 694 (1962).

[4] N. N. Bogoliubov, Izv. Akad. Nauk SSSR 11, 77 (1947); J. Phys. USSR 11, 23 (1947).

[5] N. N. Bogoliubov and D. N. Zubarev, Soviet Phys. [JETP] 1, 83 (1955).

[6] L. P. Pitaevskii and S. Stringari, *Bose-Einstein Condensates in Gases* (Cambridge University Press, Cambridge, England, 2003).

[7] E. H. Lieb, R. Seiringer and J. Yngvason, Phys. Rev. Lett. 94, 080401 (2005); A. Sütő, Phys. Rev. Lett. 94, 080402 (2005).

[8] Y. Castin and R. Dum, Phys. Rev. A 57, 3008 (1998).

[9] Ph. Nozières and D. Pines, *The Theory of Quantum Liquids* (Addison-Wesley, New York, 1990).