2

Bose systems

2.1 Generalities

In physics the concrete and traditional approach to Bose systems is to start with the Fock Hilbert space of vector states which we denote here by $\mathfrak{F}$, with a scalar product given by $(.,.)$.

Consider $L^2(\mathbb{R}^d)$, the space of square integrable functions on $\mathbb{R}^d$, $d = 1,2,...$ is the dimension of the system under consideration. Denote by $\mathscr{S}$ the space of nice (infinitely differentiable, rapid decrease) test functions in d dimension, as a subspace of $L^2(\mathbb{R}^d)$. All functions of the set $\mathscr{S}$ stand for the wave functions of the individual boson particles in the system. They are also called the *one-particle wave functions*. One considers the one-particle creation and annihilation operators with wave functions any $f,g \in \mathscr{S} \subset L^2(\mathbb{R}^d)$. The creation operator is given by $a^*(f) = \int dx f(x) a^*(x)$ acting on the space $\mathfrak{F}$. The annihilation operator is the adjoint operator of the creation operator and given by $a(f) = \int dx \overline{f}(x) a(x)$. These two operators satisfy the usual *canonical commutation relations(CCR)*

$$[a(x), a^*(y)] = \delta(x-y)\,,\ [a(x), a(y)] = 0 \tag{2.1}$$

for any $x, y \in R^d$. This leads immediately to the mathematically more complete but somewhat less popular form of the canonical commutation relations: $\forall f, g \in \mathscr{S}$ holds

$$[a(f), a^*(g)] = (f,g)\,, [a(f), a(g)] = 0 \tag{2.2}$$

It is assumed that there exists a particular normalized vector Ω in the Fock Hilbert space $\mathfrak{F}$ such that it is annihilated by all $a(x)$ and hence that: $\forall f \in \mathscr{S}$ holds

$$a(f)\Omega = 0 \tag{2.3}$$

Because of this property the vector Ω is called the *vacuum vector* of the Fock space. On the other hand the Fock space $\mathfrak{F}$ itself is taken to be the Hilbert space linearly generated by all vectors of the following set: $a^*(f_1)a^*(f_2)...a^*(f_n)\Omega$ for all $f_i \in \mathscr{S}$ and for all natural numbers $n \in \mathbb{N}$.

A.F. Verbeure, *Many-Body Boson Systems*, Theoretical and Mathematical Physics,
DOI 10.1007/978-0-85729-109-7_2,

The elements of this Fock Hilbert space are called the Fock space wave functions of the boson systems.

In this book, we use the word *state* of a boson system for each expectation valued map see Eq. (7.1) or simply for each expectation. Later we give a more detailed, more precise and more general description of this map. Nevertheless starting from the Fock Hilbert space context we describe already in a bit more details the concept of state. Let Ψ be any normalized vector, i.e. any wave function or vector of the Fock Hilbert space, then the expectation values of the type $\omega_\Psi(A) = (\Psi, A\Psi)$, where A stands for any observable of the boson system, define a *state* ω_Ψ, an expectation valued map, a map of the observables into the complex numbers.

As always the set of observables of a boson system is given by the *algebra of observables*, the algebra generated by the creation and annihilation operators.

Of course, any other representation space of the boson observables $a(x), a^*(x)$, different from the Fock space representation, yields other sets of vector states and hence other sets of states or expectation valued maps.

As said above each boson observable is expressed as a function of the boson creation and annihilation operators. In particular, each physical model is defined by giving explicitly its energy observable, called its *Hamiltonian*. For any two-body inter-particle interaction potential v, the general boson model takes the following explicit form in any finite spacial volume V, a subset of $\mathbb{R}^d$:

$$H_V = \int_V dx \frac{1}{2m} \nabla a^*(x).\nabla a(x) + \frac{1}{2}\int_V dxdy\, a^*(x)a^*(y)v(x-y)a(x)a(y) \tag{2.4}$$

where m is the mass of the particle. For simplicity of notation we put Planck's constant $\hbar = 1$. The Hamiltonian consists of the sum of two terms. The first term represents the kinetic energy of the individual boson particles of the system. The second term represents the interaction energy between the individual particles. The stability of the model requires that the Hamiltonian operator Eq. (2.4) acting on the Fock Hilbert space is bounded from below. This stability requirement puts some conditions on the potential v. Also this point is discussed later in more details.

Clearly, in order to define this Hamiltonian completely in each finite volume V, one has to specify correctly the derivatives appearing in the expression Eq. (2.4) at the boundaries of the volume. One speaks about specifying the *boundary conditions*. The problem of boundary conditions for quantum systems is a non-trivial affair. An interesting account about this topic is found in [56]. Because of the trickiness of the boundary conditions, physicists like the scheme of the *periodic boundary conditions*. In this case one takes for the finite volume sets V, the cubic boxes with sides of length L. By the same symbol V we denote as well the volume $V = L^d$ of these sets. For any such box V, one considers also the dual set V^* of the finite volume set V, namely as the set

$$V^* = \{k \in \mathbb{R}^d \,|\, k = \frac{2\pi}{L} n,\, n \in \mathbb{Z}^d\} \tag{2.5}$$

For each $k \in V^*$, denote $\varepsilon_k = k^2/2m$ and $a_k^* = V^{-1/2} \int_V dx\, e^{ik.x} a^*(x)$. Remark that the operator a_k depends in general on the volume, a property which is not indicated in the notation. In terms of this notation is the Hamiltonian Eq. (2.4) rewritten in the following form

$$H_V = \sum_{k \in V^*} \varepsilon_k a_k^* a_k + \frac{1}{2V} \sum_{k,k',q} v(q) a_{k+q}^* a_{k'-q}^* a_{k'} a_k \tag{2.6}$$

where $v(q)$ stands now for the Fourier transform of the potential v.

A many-body physicist is interested to know basically everything about all the properties of the systems defined by the Hamiltonian Eq. (2.6). He is interested in the spectra, the dynamics, the ground states, the equilibrium states, etc ... etc. Unfortunately the nasty aspect of this general model is that it is in general not a solvable system. Not its ground states nor its equilibrium states (see next Chapter) have ever been rigorously computed for a non-trivial potential function v.

Essentially, a system is often called solvable if one can construct an expectation valued map or a state $\widetilde{\omega}$ which is the ground state or the equilibrium state at a certain temperature of the system H_V for some volume V or in the limit V (or L) tending to infinity. In the rest of the book we use the notation $\lim_V$ in order to indicate this limit. This limit is always referred to as the *thermodynamic limit*. A more precise and complete technical definition of solvability comes later.

For a boson system, as all observables are build up by means of the creation and annihilation operators and because of the canonical commutation relations, a particular expectation valued map or a state, say $\widetilde{\omega}$, is known if one knows all its *correlation functions*, i.e. if one knows all the expectation values of the type

$$\widetilde{\omega}(a^*(f_1)...a^*(f_n)a(g_1)...a(g_m)) \tag{2.7}$$

for all functions $f_i, g_j \in \mathscr{S}$ and for all pairs $n,m \in \mathbb{N}$. One should realize that in order to know the state one has to know or to specify an infinity of correlation functions, one for each pair (n,m). The expression given by (2.7) is called the *(n,m)-correlation function* or the *correlation function of order n+m*. Clearly there are in general infinitely many different correlation functions.

This infinity can make the problem of solving an interacting boson system infinitely difficult. This is the origin of the expression, a boson system with a non-trivial potential is in general non-solvable. This infinity is also the main reason for the fact that the search for solvable models is a genuine occupation for many researchers working in many-body boson systems.

In the physics literature one finds many approximation procedures which consist of reducing this infinity of different correlation functions of a ground state or of an equilibrium state to a finite number of independent ones. Many of them consist of different decoupling suggestions of arbitrary (n,m)-correlation functions Eq. (2.7). For instance, a lot of these proposed approximation procedures are of the type of assuming that all higher order correlation functions, say of order larger than $n+m$, can be expressed in terms of those of lower orders, say less than $n+m$. It must be remarked that, on the basis of the theorem of Marcinkiewicz [146], many of them are erroneous in the sense that such decoupling procedures may contradict the positivity (see further) of the state $\widetilde{\omega}$. In fact this theorem tells us something very important. It tells us that the only valid decoupling procedure is the following. If the decoupling holds for all correlation functions from some order $n+m$ on, then the decoupling holds for all correlation functions of all orders $n+m>2$. This means that the only mathematically rigorous and physically meaningful decoupling, not contradicting the positivity of the state $\widetilde{\omega}$, is the decoupling whereby the state is given in terms of the one- and two-point functions, which are in finite number and given by the following: for all f,g: $\widetilde{\omega}(a(f)), \widetilde{\omega}(a^*(f)a(g)), \widetilde{\omega}(a(f)a(g))$. In other words this means that in general, any state is determined by a fixed finite number, maximum three, of correlation functions or by an infinity of them. Or stated in general, any state is, or determined by its one and two-point correlation functions, or by an infinity of different correlation functions. All intermediate cases are contradicting the positivity property of the state as an expectation valued map.

Of course, the most representative example of a state determined by its one and two-point functions is the so-called the *Fock state* ω_F or the Fock expectation valued map $\omega_F(A) = (\Omega, A\Omega)$, satisfying (2.3). It is an instructive student exercise to check the decoupling property for the Fock state. As is well known, the Fock state yields the ground state (see also further on) of the free boson gas (see Eq. (2.4) with $v=0$).

Furthermore any state satisfying the correct decoupling procedure which is described above will be called a *quasi-free state* and any boson model whose ground state is given by such a quasi-free state shall be called a *solvable model*. More complete and more elaborate definitions of these two important notions are explained in more details below.

The rest of this chapter is devoted to the essentials of the boson canonical commutation relations, to its set of space homogeneous states, its gauge invariant states and its subset of quasi-free states. The latter ones will be very practical for the formulation of the variational principles of statistical mechanics for solvable models. The more mathematically minded reader can find more general and more sophisticated treatments of some of the material in [131] and [26].

2.2 CCR and boson fields

We introduced the creation and annihilation operators $a^\sharp$ acting on the Fock space $\mathfrak{F}$ where the symbol $\sharp$ refers either to the creation operator or to the annihilation operator. In order to define the total set of states as well as the set of all quasi-free states it is sometimes handy to work with the notion of boson fields.

The *boson field* is given by the map $b : f \in \mathscr{S} \subseteq L^2(\mathbb{R}^d) \to b(f)$, where

$$b(f) = a(f) + a^*(f) \tag{2.8}$$

Clearly each $b(f)$ is a self-adjoint linear operator on the Fock Hilbert space. In the physics literature, $\mathscr{S}$ is also called a space of test functions consisting of the infinitely differentiable functions with rapid decrease at infinity. Remark that the creation operators are complex linear on the space of test functions $\mathscr{S}$, the annihilation operators are complex anti-linear, and therefore the fields are only real linear in their arguments, one computes e.g. $b(if) = i(-a(f) + a^*(f))$ and therefore $a(f) = \frac{1}{2}((b(f) + ib(if))$.

The *canonical commutation relations* (2.2) translated in terms of the fields take now the form

$$[b(f), b(g)] = 2i\sigma(f,g) \tag{2.9}$$

with $\sigma(f,g) = \Im(f,g)$. Remark that σ is a real bilinear antisymmetric form on the real test-function space $\mathscr{S}$. Such a form on a real vector space is called in general a *symplectic form* and any real linear space equipped with a symplectic form is called a *symplectic space*. Hence the couple $(\mathscr{S}, \sigma)$ realizes a symplectic space. The reader understands from Eq. (2.9) that the canonical commutation relations in terms of the fields are completely determined solely by such a symplectic form σ. This conclusion holds as well for the next formulation of the commutation relations.

Clearly, working with the field operators as the generators of all observable quantities or working with creation and annihilation operators are equivalent procedures.

It is also clear that both sets of generators, as well the fields as the creation-annihilation operators, consist of unbounded operators. For many mathematical manipulations and argumentations working with bounded operators has its technical mathematical advantages. Therefore, but also for other technical reasons, Weyl proposed to use the following unitary operators as the generators of all the observable quantities of boson systems. For any $f \in \mathscr{S}$ the corresponding *Weyl operator* is given by the unitary operator

$$W(f) = exp\{ib(f)\} \tag{2.10}$$

Using the well known Baker-Campbell-Hausdorff formula argument, telling that for the operators X and Y, both commuting with the commutator $[X,Y]$, holds

$$e^X e^Y = e^{X+Y} e^{\frac{1}{2}[X,Y]}$$

one derives from (2.9) that the canonical commutation relations Eq. (2.2) in terms of the Weyl operators get the following form:

$$W(f)W(g) = W(f+g)e^{i\sigma(f,g)} \tag{2.11}$$

It should be clear that algebraically, i.e. up to a number of topological aspects which we disregard here, one has now the option to work with three different presentations of the *boson algebra of observables* $\mathfrak{A}$, namely:

(i) the algebra generated by the creation and annihilation operators and the unit operator,

(ii) the algebra generated by the fields and the unit operator, or

(iii) the algebra generated by all the Weyl operators.

The latter one is of course the most suitable one for the research in pure mathematical physics and is very much used in the field called the algebraic approach to statistical mechanics and field theory. The two other presentations are mostly used by theoretical physicists as is also well known. A rather complete account of all this can be found in [26].

So far for the *algebra of observables*, which we denote simply by $\mathfrak{A}$ for any of the tree settings.

2.3 States and Quasi-Free States

We discuss the set of states on the algebra of observables $\mathfrak{A}$. As indicated above, a state on the algebra $\mathfrak{A}$ is an expectation valued map.

Definition 2.1. *The mathematical properties of any state ω are the following: it is a normalized-to-one, linear, positive form or functional on the algebra of observables $\mathfrak{A}$. More explicitly, the state ω maps each observable $A \in \mathfrak{A}$ into its expectation value which is in general a complex number $\omega(A)$ with the properties*

(i) normalization: $\omega(1) = 1$

(ii) linearity: for each pair A, B of observables and each pair λ, μ of complex numbers one has $\omega(\lambda A + \mu B) = \lambda\, \omega(A) + \mu\, \omega(B)$

(iii) positivity: for each observable A holds the positivity of the expectation value $\omega(A^* A) \geq 0$

It is perhaps important to realize that these are indeed the essential properties that a state ω should have in order to give to the expression $\omega(A)$ the interpretation of the expectation value of an observable A as we learned about in our undergraduate lectures. For these reasons it is clear that the notion of state is indeed a mathematical formalization of the notion of expectation valued map. The notion of state has a direct link to the notion of observation values in quantum physics and is therefore much more to the point than the notion of wave function. Remark that in our language the notion of state is not the same as the one which one finds in standard books on quantum mechanics, where a state is a vector, called the wave-function, an element of a Hilbert space, which itself can be referred to as the set of vector-states. The link between the notion of vector-state or wave function, and our more general notion of state, is mathematically realized by the so-called *GNS-construction* (see [26] and (7.1)), which is a very general and important theorem telling us the following. Let ω be any state on the algebra of observables $\mathfrak{A}$, then there exists a representation π of the canonical commutation relations algebra acting on a Hilbert space $\mathscr{H}$ and a special vector, called *cyclic vector*, Ω in $\mathscr{H}$ such that $\omega(X) = (\Omega, \pi(X)\Omega)$ for any observable X. We should immediately remark that the Hilbert space $\mathscr{H}$ needs not to coincide with the original Fock space. One knows more. One knows that in most physically interesting cases they do not coincide. The reader does understand that our notion of state does create a generality concerning expectation values which is going far beyond the Fock space. It turns out that this generality is necessary in order to understand the most interesting phenomena about systems with a large(=infinite) number of degrees of freedom. This is the main reason for our choice of working with the notion of state or expectation valued map in stead of with wave functions.

Denote by $\mathscr{E}$ the *set of states* on the boson observable algebra. First of all it is interesting to remark that this set $\mathscr{E}$ is a convex set, i.e. for each pair of states ω_1, ω_2 and each real number λ in the interval $[0,1]$, also the convex combination $\omega = \lambda\, \omega_1 + (1-\lambda)\, \omega_2$ is again a state. It is clear that the value of λ has the physical interpretation of the concentration of the state ω_1 in the state ω and $1-\lambda$ the concentration of ω_2 in the state ω. This remark leads to the following notions. A state is called a *pure state* or an *extremal state*, if it is not possible to write the state as a non-trivial convex combination of two other different states. Hence the state ω is pure if $\omega = \lambda\,\omega_1 + (1-\lambda)\,\omega_2$ implies $\lambda = 0$ or $\lambda = 1$, and/or implies $\omega_1 = \omega_2$. A state is a *mixed state* if it is not a pure state. Of course the notion of convex combination of finite sums extends straightforwardly to infinite sums and even to integrals of states. In particular the following situation will be relevant for us. Consider any convex set S of a vector space equipped with a probability measure μ (i.e. for $\lambda \in S$, $\mu(\lambda) \geq 0$, $\int d\mu(\lambda) = 1$) defined on S. Let $\{\omega_\lambda\}$ be a set of states labeled by the parameter λ, then also the integral $\omega = \int d\mu(\lambda)\omega_\lambda$ is again a state, because the set of states $\mathscr{E}$ is a convex set.

Now we look for a general but practical definition of the set of states for boson systems also with the intention to formulate clearly the particular subset of states which will be called the set of quasi-free states. For these aims the Weyl formulation is very suitable.

Let ω be an arbitrary state on the Weyl algebra $\mathfrak{A}$. This state is known or well defined, if for all $f \in \mathscr{S}$, all the expectation values $\omega(W(f))$ are known, or if the expectation values of all Weyl operators are known. A straightforward classical computation (see e.g. [146]) yields the expression of the expectation values in terms of the field correlation functions

$$\begin{aligned}\omega(W(f)) = \omega(e^{i\lambda b(f)}) &= \sum_{n=0}^{\infty} \frac{i^n \lambda^n}{n!}\omega(b(f)^n) \\ &= \exp\{\sum_{n=1}^{\infty} \frac{i^n \lambda^n}{n!}\omega(b(f)^n)_t\}\end{aligned} \tag{2.12}$$

where the so-called *truncated correlation functions* $\omega(\ldots)_t$ are defined recursively through the formula

$$\omega(b(f_1)\ldots b(f_n)) = \sum \omega(b(f_k)\ldots)_t \ldots \omega(\ldots b(f_l))_t \tag{2.13}$$

where the sum is over all possible partitions $(k,\ldots),(\ldots),\ldots(\ldots l)$ of the set $\{1,\ldots,n\}$, with the order within each of the clusters carried over from the left to the right hand side. Because of this definition, one calls each $\omega(b(f_1)\ldots b(f_n))_t$ the truncated correlation function of order n. In the physics literature the word "connected" is also sometimes used in stead of the connotation "truncated".

The formula Eq. (2.12) expresses that the state is completely defined if one knows all its truncated correlation functions and vice versa.

In this Weyl formulation the basic properties of a state are now explicitly given by: let $A = \sum_i c_i W(f_i)$ be any arbitrary element of the algebra of observables, then

(i) normalization: $\omega(W(0)) = \omega(1) = 1$

(ii) linearity: $\omega(A) = \sum c_i\,\omega(W(f_i))$

(iii) positivity: $\omega(A^*A) \geq 0$

This completes the definition of a general state on the algebra of boson observables in terms of the field correlation functions or equivalently in terms of the truncated field correlation functions.

Now we are able to identify a very special class of states, namely the set of quasi-free states.

Definition 2.2. *A state ω of the boson algebra of observables is called a quasi-free state, also written qf-state, if all its truncated correlation functions of all orders $n > 2$ vanish. This has the immediate consequence that all its $(n > 2)$-correlation functions are expressed in terms of those of orders $n \leq 2$.*

From the formula Eq. (2.12) it follows that the most general quasi-free state is completely determined by its one- and two-point correlation functions and therefore gets the following simpler explicit form:

$$\omega(W(f)) = \exp\{i\omega(b(f)) - \frac{1}{2}\omega(b(f)b(f))_t\} \tag{2.14}$$

We denote by $\mathfrak{Q}$ the set of all quasi-free(qf) states. Some authors call the set of quasi-free states also the set of generalized free states.

Remark that, if one takes any real linear functional $\chi : f \rightarrow \chi(f)$ on the test function space $\mathscr{S}$, then any such functional defines a *canonical transformation* Eq. (7.3) τ_χ, i.e. a one-to-one transformation mapping the observables onto the observables leaving the canonical commutation relations (CCR) invariant. It is acting on the boson algebra $\mathfrak{A}$ in the Weyl form as follows

$$\tau_\chi(W(f)) = e^{i\chi(f)}W(f) \tag{2.15}$$

together with the rules that τ_χ is linear, conserves all products as well as the *-operation. Note that the composition of any state ω with the canonical transformation τ_χ, i.e. that $\omega \circ \tau_\chi$, is again a state.

It is immediately checked from Eq. (2.15) that the action of this transformation is nothing else but translating the boson fields with a scalar quantity, namely: $\tau_\chi b(f) = b(f) + \chi(f)$. This follows directly from the formal computation

$$\frac{d}{d\lambda}\tau_\chi(W(\lambda f))|_{\lambda=0} = e^{i\lambda\chi(f)}W(\lambda f)|_{\lambda=0}$$

Take any qf-state ω Eq. (2.14), then the composition $\widetilde{\omega} = \omega \circ \tau_\chi$ is not only again a state, one readily checks that it is again a qf-state. In particular if one chooses $\chi(f) = -\omega(b(f))$ then the one-point function of the new state $\widetilde{\omega}$ vanishes. Moreover the two-point truncated function is left invariant for the transformation τ_χ, i.e. $\widetilde{\omega}(b(f)b(g))_t = \omega(b(f)b(g))_t$. Therefore, up to such a canonical transformation, one can continue the analysis of the set of qf-states with the set of qf-states restricting ourself to those with vanishing one-point function. In this case the definition of qf-state Eq. (2.14) reads as follows

$$\omega(W(f)) = \exp\{-\frac{1}{2}\omega(b(f)b(f))\} \tag{2.16}$$

because in this case $\omega(b(f)b(g))_t = \omega(b(f)b(g))$.

Denote $s(f,f) = \omega(b(f)^2)$ then Eq. (2.16) becomes

$$\omega(W(f)) = \exp\{-\frac{1}{2}s(f,f)\} \tag{2.17}$$

Denote also by $s(f,g)$ defined on $\mathscr{S} \times \mathscr{S}$, the real bilinear symmetric extension of $s(f,f)$ on $\mathscr{S}$. By differentiating twice $\omega(W(\lambda f)W(\mu g))$ with respect to λ and μ at zero, one obtains the two-point function for the fields in the following form

$$\omega(b(f)b(g)) = s(f,g) + i\sigma(f,g) \tag{2.18}$$

The positivity condition applied to the qf-state ω becomes: for all $A = \sum c_i W(f_i)$ holds

$$\begin{aligned} 0 \leq \omega(AA^*) &= \sum_{j,k} c_j \overline{c_k}\, \omega(W(f_j - f_k)) \exp(-i\sigma(f_j, f_k)) \\ &= \sum_{j,k} (c_j e^{-\frac{1}{2}s(f_j,f_j)})(\overline{c_k} e^{-\frac{1}{2}s(f_k,f_k)}) \exp(s(f_j,f_k) - i\sigma(f_j,f_k)) \\ &= \sum_{j,k} d_j \overline{d_k} \exp(s(f_j,f_k) - i\sigma(f_j,f_k)) \end{aligned}$$

where the parameters d_k are immediately identified from the second line. Use the following general matrix property which is straightforwardly checked. If the matrices $A = (a_{i,j})$ and $B = (b_{i,j})$ are positive definite $n \times n$-matrices, then the matrix $C = (a_{i,j} b_{i,j})$ is also a positive definite matrix (see e.g. [131]). This property yields immediately the proof of the fact that the positivity of the qf-state is equivalent to the positive definiteness of the two-point function Eq. (2.18). Expressed in words, the positivity of a qf-state ω restricted to the monomials in the fields of order two, is necessary and sufficient for the full positivity of the qf-state.

All field correlation functions can as well be expressed in terms of the creation and annihilation operators (n,m)-correlation functions Eq. (2.7) and vice versa. Therefore one can express as well, and equivalently, this positivity in terms of the creation and annihilation operators $a^\sharp$ which are complex linear, respectively anti-linear in the test functions. The positivity of the quasi-free state ω is therefore expressed by: $\forall f,g \in \mathscr{S}$, considered now as a complex linear space, the positivity of the state becomes

$$\omega((a(f) + a^*(g))(a(f) + a^*(g))^*) \geq 0 \tag{2.19}$$

This is indeed the necessary and sufficient condition for the positivity of the state.

The next step in the analysis of the states of boson systems is by introducing the parameterizations of the truncated two-point functions of any state ω by means of operators. In the following we consider states for which the truncated two-point functions are determined by the (unbounded) operators R and S acting on the space $\mathscr{S}$, and which are defined as follows

$$\omega(a(f)a^*(g))_t = (f, Rg)\,; \;\; \omega(a(f)a(g))_t = (f, S\overline{g}) \tag{2.20}$$

where the symbol $\overline{g}$ stands for the complex conjugate of g. Clearly the symbol $(.,.)$ stands for the scalar product on $L^2(\mathbb{R}^d)$.

It is important to note that this operator presentation holds for the truncated two-point correlation functions of any state, being quasi-free or not. Moreover, an identical operator representation of any truncated (n,m)-correlation function (see

Eq. (2.7) or Eq. (2.13)) can be obtained by an operator mapping any dense subspace of $L^2(\mathbb{R}^{dn})$ into $L^2(\mathbb{R}^{dm})$.

In particular for quasi-free states, as all higher $(n+m>2)$ order truncated correlation functions vanish, one can rewrite the full positivity condition Eq. (2.19) of a quasi-free state solely in terms of the operators R and S, defined in Eq. (2.20). The reader realizes that the positivity conditions of a general state involve however all correlation functions of all orders.

Before continuing the analysis of the positivity conditions, it may be instructive to illustrate first the material by making a small intermezzo presenting a couple of well known examples of states and quasi-free states in terms of their operator presentation. After that we concentrate ourself onto the subclasses of all states which are space homogeneous or space translation invariant and gauge invariant.

Examples of boson systems states

The notion of quasi-free state is not so mysterious as it may sound. The examples used all around in the physics literature are daily matters. As already mentioned, the best known example of a quasi-free state is the *Fock state* ω_F given by: for all $f \in \mathscr{S}$,

$$\omega_F(W(f)) = (\Omega, W(f)\Omega) = e^{-\frac{1}{2}(f,f)} \tag{2.21}$$

where Ω is the vacuum wave vector of the Fock Hilbert space Eq. (2.3). The GNS-representation space (7.1) of the Fock state is the Fock Hilbert space $\mathfrak{F}$ and the cyclic vector is the vacuum vector Ω. In other words the Fock state is the expectation valued map determined by the Fock vacuum vector. From Eq. (2.21) it follows that the defining operators (R,S) Eq. (2.20) of the Fock state ω_F are given by the operators $R = 1$ and $S = 0$. Furthermore the one-point function of the Fock state vanishes.

A subset of the set $\mathfrak{Q}$ of qf-states, is the set of so-called *coherent states* associated to the Fock state ω_F. Denote this set of coherent states by $C(\omega_F)$. This set of states is given by all states $C(\omega_F) = \{\omega_h\,;\, h \in \mathscr{S}\}$ where the ω_h are defined by the formulae

$$\omega_h(W(f)) = (W(h)\Omega, W(f)W(h)\Omega) = (\Omega, W(f)\Omega)e^{i2\sigma(f,h)} = \omega_F \circ \tau_\chi(W(f)) \tag{2.22}$$

with τ_χ again the canonical transformation Eq. (7.3) of the field translations with $\chi(f) = 2\sigma(f,h) = 2\Im(f,h)$. In particular it is clear that all states of the set $C(\omega_F)$ are build on the ground state wave function or the Fock vacuum wave vector Ω. It is also clear that all coherent states ω_h, associated with the Fock state, are quasi-free states of the boson systems.

However it is also clear that the notion of coherent state can be associated to any other state ω of the boson algebra of observables $\mathfrak{A}$. The set of coherent states $C(\omega)$ associated with the state ω is analogously given by $C(\omega) = \{\omega \circ \tau_\chi \,|\, \forall \chi(f) = 2\Im(f,h), h \in \mathscr{S}\}$. If ω is a qf-state then the set $C(\omega)$ is a subset of the qf-states. However, if ω is not a qf-state, then none of the states of $C(\omega)$ are qf-states. Hence the notion of coherence for a state is not necessary linked to the notion of quasi-freeness. If one considers the GNS-representation of the state ω: $\omega(X) = (\Psi, X\Psi)$

with cyclic vector Ψ, then this vector is the ground wave function of all states in the set $C(\omega)$. A priori this vector need not to be an element of the Fock Hilbert space $\mathfrak{F}$.

Needless to mention that the notion of coherent state has been used in many applications in physics. For instance, most of the exact results concerning the settings and the derivations of different forms of the Hartree-Fock equations [159] are obtained using the coherent state technology. It is clear that in all these applications, a main starting point consists of making the best choice for the generating state ω or of the right choice for the ground state wave function. Next to the coherent state idea and technology, there is also the wavelet state technology, which can be considered as a generalization of the coherent state technology. We do not enter here into the details about the wavelet states, because their applications are so far not too much present in many body boson physics.

Homogeneous states

The space translations are again realized by a group of canonical transformations Eq. (7.3) $\{\tau_x | x \in \mathbb{R}^d\}$ acting on the algebra of observables $\mathfrak{A}$ and are given by the maps $\tau_x(a(f)) = a(T_x f)$ where T_x is the action of translation over the distance x (7.3), $(T_x f)(y) = f(y-x)$, acting on the test function space $\mathscr{S}$.

Definition 2.3. *The set of homogeneous states or space translation invariant states is given by all states ω which satisfy the following invariance property: for all $x \in \mathbb{R}^d$ holds $\omega \circ \tau_x = \omega$.*

Let us illustrate an immediate implication of the homogeneity of a state on the correlation functions.

Using the fact that $\tau_x a_k = \frac{1}{\sqrt{V_x}} \int_{V_x} dy\, a(y) e^{-ik(y-x)} = e^{ikx} \frac{1}{\sqrt{V}} \int_{V_x} dy\, a(y) e^{-iky}$, with $V_x = V + x$, one gets $\lim_V \omega(\tau_x(a_k)) = e^{ikx} \lim_V \omega(a_k)$. Hence, if the state ω is homogeneous, one gets that for all $k \neq 0$, $\lim_V \omega(a_k) = 0$ in the thermodynamic $\lim_V$. Check that for homogeneous states ω holds in general $\lim_V \omega(a^*_{k_1} \ldots a^*_{k_n} a_{k_{n+1}} \cdots a_{k_{n+m}}) = 0$ if $k_1 + \ldots + k_n - k_{n+1} - \ldots . - k_{n+m} \neq 0$.

Furthermore supposing that ω is a space translation invariant state, and using the operator representation of the two-point truncated functions Eq. (2.20), one gets that the invariance property is transported to the operators R, S with the property that both operators R and S commute with all the operators T_x, because e.g. for all x holds

$$\begin{aligned}(f, Rg) &= \omega(a(f)a^*(g)) = \omega(\tau_x(a(f)a^*(g))) \\ &= \omega(a(T_{-x}f)a^*(T_x g)) = (f, T_{-x} R T_x g)\end{aligned}$$

and therefore $[R, T_x] = [S, T_x] = 0$. Operators with these properties are sometimes called translation invariant operators.

It is a fairly well known property [78] that if A is any such translation invariant operator, then there exists a tempered distribution on the test function space $\mathscr{S}$ with Fourier transform a function ξ such that for all functions f with Fourier transform $\widehat{f}$ holds $\widehat{Af}(p) = \xi(p)\widehat{f}(p)$. This means that the operator A is a simple multiplication operator. This property is a consequence of the kernel theorem for operator valued distributions and the convolution theorem for Fourier transforms. In the following, for notational convenience, we omit the notation for Fourier transforms and write simply

$$Af(p) = \xi(p)f(p) \tag{2.23}$$

In any case for homogeneous states, the two-point correlation function operators R and S are simply multiplication operators with functions which we denote by $r(p)$, respectively $s(p)$. It is easily checked from Eq. (2.20) that $r(p) = \omega(a(p)a^*(p))$ and $s(p) = \omega(a(p)a(-p)) = s(-p)$ where the $a(p)^\sharp$ are the usual operator valued distributions, the Fourier transforms of the creation and annihilation operators $a^\sharp(x)$ introduced before. For our purposes, as we consider only time reversal invariant systems, we can as well assume from now on that also the r-function is a symmetric function of its argument p: $r(-p) = r(p)$.

As all multiplication operators are two by two commuting with each other, also the operators R and S commute with each other: $[R,S] = 0$.

Analogously as for the two-point truncated correlation functions of a translation invariant state, all its truncated higher order (n,m)-correlation functions can be described by analogous multiplication operators with functions in $n+m-1$ variables. The positivity of the state does imply of course a number of necessary and sufficient conditions on these functions. We do not write out in full details all these conditions for all the (n,m)-correlation functions of orders $n+m>2$.

On the other hand we apply this result to the set of homogeneous quasi-free states. For these states, from the analysis given above, one can conclude that any qf-state ω with vanishing one-point function is completely and equivalently labeled by the operators R,S as well as by its associated functions r,s. Therefore the qf-state is uniquely denoted as $\omega_{(R,S)}$ as well as by $\omega_{(r,s)}$.

Now we are in a position to express the necessary and sufficient positivity conditions of a space homogeneous qf-state ω explicitly in terms of its determining operators or its corresponding multiplication functions. Writing out the positivity condition Eq. (2.19) yields: $\forall f,g$,

$$0 \leq (f,Rf) + (f,S\Lambda g) + \overline{(f,S\Lambda g)} + (g,(R-1)g)$$

where Λ is the conjugation operator with the property: $(\Lambda f, \Lambda g) = (g,f)$. Remark first that the special case $f=0$ yields already the following condition on the operator R, namely: $R \geq 1$. In particular it follows that the operator R is self-adjoint. Using this property one gets $(\Lambda g,(R-1)\Lambda g) = (g,(R-1)g)$ and $\overline{(f,S\Lambda g)} = (\Lambda g, S^* f)$, and one obtains, with Λg replaced by g, the positivity conditions in the following form

$$0 \leq (f,Rf) + (f,Sg) + (g,S^*f) + (g,(R-1)g)$$

which are immediately translated into the equivalent operator or function conditions:

$$0 \leq R(R-1) - S^*S \tag{2.24}$$

$$0 \leq r(p)(r(p)-1) - |s(p)|^2 \tag{2.25}$$

This form of the positivity conditions suggests the introduction of the following non-negative function $t(p)$, defined by $t(p)^2 = r(p)(r(p)-1) - |s(p)|^2$, expressing the full positivity of the qf-state determined by the functions (r,s). Therefore the qf-state can now better be labeled by the functions $r \geq 1, t \geq 0$ and the real number $\alpha = \arg s$. Hence in the rest of this text we may label equivalently the qf-state ω with vanishing one-point function by $\omega_{R,S}$ or as well by $\omega_{(r,t,\alpha)}$. One should remember that in this notation it is pre-supposed that the one-point function is put equal to zero. If this is not equal to zero, one should get a full parametrization only if also the one-point parameter is added to the notation. For translation invariant states we use the one-point parameter c, defined by $c\widehat{f}(p=0) = \omega(a^*(f))$, which makes sense again as an immediate consequence of the homogeneity of the state. Hence a full parametrization of a qf-state looks as follows: $\omega_{c,r,t,\alpha}$.

Ergodic states

Definition 2.4. *Consider any general homogeneous or space translation invariant state ω, i.e. a state satisfying, for all $x \in \mathbb{R}^d$, the equality $\omega \circ \tau_x = \omega$. The state is called an extremal space invariant or ergodic state, if for each pair (A,B) of local observables, i.e. build up by creation and annihilation operators $a^*(f), a(f)$ with test-functions $f \in \mathscr{S}$ of finite local support, holds*

$$\lim_{|x|\to\infty} \omega(A\tau_x B) = \omega(A)\,\omega(B) \tag{2.26}$$

Notice that an ergodic state is always a space invariant or homogeneous state. The property of ergodicity of a state means that the expectation value of the product of two observables equals the product of the expectation values of each of them if one of the observables is moved far away. It means also that the state has a kind of asymptotic product property or an asymptotic independence property. Remark that ergodic states have an interesting property concerning the expectation values of space averages of observables. Indeed, let A,B,C be arbitrary local observables, and consider the expression $\lim_V \omega(AB_V C)$, where $B_V = \frac{\int_V dx\,\tau_x B}{V}$ with τ_x again the space translation over the distance x. Hence B_V is the operator B averaged over the space volume V. For any fixed finite volume V_0 holds

$$\lim_V \omega(AB_V C) = \lim_V \omega(A(\frac{\int_{V_0} dx\,\tau_x B}{V} + \frac{\int_{V-V_0} dx\,\tau_x B}{V})C)$$

Because $\lim_V (V_0/V) = 0$, the first term vanishes. Looking at the second term, take the volume V_0 such that it contains the support of the local operator C. Then the operator C commutes with the integral on the basis of the locality of the canonical commutation relations. Finally using the ergodicity of the state one gets the formula

$$\lim_V \omega(AB_V C) = \omega(AC)\omega(B) \tag{2.27}$$

Without going into too much mathematical details, this means that the space average operator $\lim_V B_V$ exists and is equal to the expectation value $\omega(B)$ of the operator B

multiplied by the unit operator i.e. $\lim_V B_V = \omega(B)1$. Notice the explicit dependence of this limit on the state. In mathematics the type of limit considered in Eq. (2.27) goes under the name of weak operator limit. For more technical details about the mathematics of ergodic states one may consult [26].

Furthermore, for later applications, it is essential to mention the following relation between homogeneous states and ergodic states. In particular there is a theorem (for all mathematical details see [26] Volume I, Chapter 4) telling essentially that each space translation invariant state can be written as a convex sum of ergodic invariant states. In more explicit formulae, let $\{\omega_\lambda | \lambda \in E\}$, with λ some parameter of a convex set E, be the set of ergodic states and ω an arbitrary homogeneous state, then there exists always a probability measure μ, defined on the parameter set E, such that $\omega = \int d\mu(\lambda)\, \omega_\lambda$. This means that each homogeneous state can written as a convex combination of ergodic states. In more down to earth words, it means that if one knows all ergodic states satisfying some physical property linear on the set of the homogeneous states, one can check what it means for all the homogeneous states.

Clearly the notion of ergodicity which is introduced, is related to the non-compact invariance group, namely the complete translation group $\mathbb{R}^d$. It is clear that in the definition of ergodicity, the group $\mathbb{R}^d$ can be replaced by any infinite non-compact subgroup. Important subgroups are for instance the subgroups $\mathbb{G}$ of the translations over sublattices of the full translation group $\mathbb{R}^d$.

There exist general theorems about the question, when can a state, ergodic for the full group, be written as a convex combination of states which are ergodic for a subgroup $\mathbb{G}$. In all this it is however important to realize the fact that the notion of ergodicity is always linked to a specific infinite translation group.

All these mathematical theorems as such will not be used in the later applications. On the other hand, some of these properties will directly be derived in different physical boson systems applications.

Finally we mention that the notion of ergodic state is a rigorous mathematical notion for what in physics is sometimes called a *pure phase state*. For this reason, ergodic states are also sometimes called *extremal invariant states*. Let us mention here at least one of the applications of the decomposition theorem of an invariant state into its ergodic or extremal components, namely the decomposition into the ergodic states with respect to a non-trivial subgroup. This type of decomposition shall lead us to the main concept of the analysis of the phenomenon of spontaneously broken symmetries, discussed for boson systems in full details in Chapter Eq. (4). The reader should be aware that the notion of spontaneous symmetry breaking is an important item not only within the domain of Bose-Einstein condensation, but in fact in many more other modern theories in physics running from solid state physics over low energy nuclear physics up to high energy physics. In any case it comes over as a a phenomenon which is typical for all systems with a large or an infinite number of degrees of freedom.

Homogeneous quasi-free states and their ergodicity

Now we look for the ergodicity properties of space homogeneous qf-states. Take any homogeneous qf-state ω. In terms of the Weyl operators, we check the ergodicity condition and therefore consider the limit $|x| \to \infty$, for all local functions (functions of compact support) f, g with $g_x(y) = g(y-x)$, of the two-point functions with $A = W(f)$ and $B = W(g)$. First compute the relation for a qf-state

$$\omega(A\,\tau_x B) = \omega(W(f)\tau_x W(g)) = \omega(W(f))\omega(W(g))\exp\{i\sigma(f,g_x) - s(f,g_x)\}$$

On the basis of the Riemann-Lebesgue Lemma one gets $\lim_{|x|\to\infty}\sigma(f,g_x) = 0$, as well as $\lim_{|x|\to\infty} s(f,g_x) = 0$, and the following properties of the two-point functions

$$\lim_{|x|}\omega(a(f)a^*(g_x))_t = \lim_{|x|}\int dp\, r(p)\overline{f(p)}e^{ip.x}g(p) = 0$$

$$\lim_{|x|}\omega(a(f)a(g_x))_t = \lim_{|x|}\int dp\, s(p)\overline{f(p)}e^{-ip.x}\overline{g(p)} = 0$$

Hence the two-point functions share the ergodicity property. Looking at the one-point function, one gets from the space translation invariance $\omega(\tau_x a(f)) = \omega(a(f))$ for all x, implying that the one-point function is, as pointed out above, of the form $\omega(a^*(f)) = cf(0)$ where c is some complex constant.

In any case, all this shows that each space homogeneous or space translation invariant qf-state has always the property of being an ergodic state.

In this context, it is also important to remark that any non-trivial convex combination of two different homogenous qf-states is never a qf-state. In particular this means that by taking convex combinations of qf-states one generates a new class of states which are not anymore quasi-free states. It must be recognized that a deeper characterization and understanding of the structure of this set of generated states has so far not been cleared up. It remains a challenging open problem to get a better knowledge concerning the most intrinsic mathematical and physical properties common for all convex compositions of qf-states.

Gauge invariance

Finally we consider one more group of canonical transformations Eq. (7.3) of the CCR-algebra of observables, namely the *gauge transformations group* $\{\tau_\lambda | \lambda \in [0,2\pi] \subset \mathbb{R}\}$ Eq. (7.3), defined by the operations

$$\tau_\lambda(a^*(f)) = e^{i\lambda}a^*(f),\ \tau_\lambda(a(f)) = e^{-i\lambda}a(f) \tag{2.28}$$

The reader checks easily that also these transformations leave the canonical commutation relations invariant. One verifies that this group is isomorphic to the additive group modulo 2π of the real numbers $[0,2\pi]$ and therefore coincides with the compact unitary group commonly denoted by $U(1)$.

Definition 2.5. *Any boson state ω is called gauge invariant, if for all $\lambda \in [0,2\pi]$ holds that $\omega \circ \tau_\lambda = \omega$.*

It is immediately clear from the definition that for any gauge invariant state ω all (n,m)-point correlation functions with $n \neq m$ vanish. In particular all odd-point($n+m = odd$) correlation functions vanish. In particular the one-point function vanishes.

Let us now look closer at the action of the gauge transformations on qf-states and characterize the gauge invariant qf-states. In terms of general states we confine our attention to the one and two-point functions of a state. If the state is gauge invariant, we remarked already that the one-point function vanishes. In that case looking at the two-point functions, clearly a qf-state $\omega_{(R,S)}$ transforms under a gauge transformation as follows: $\omega_{(R,S)} \circ \tau_\lambda (a(f)a^*(g)) = \omega_{(R,S)}(a(f)a^*(g))$ and $(\omega_{(R,S)} \circ \tau_\lambda)(a(f)a(g)) = e^{-i2\lambda}(\omega_{(R,S)})(a(f)a(g))$ or equivalently the operator pair (R,S) is changed into the pair $(R, e^{-i2\lambda}S)$.

Therefore the qf-state $\omega_{(R,S)}$ or in general the two-point functions of an arbitrary state are gauge invariant if and only if the operator S vanishes, i.e. if and only if the two-point functions of the state are of the form $\omega_{(R,S=0)}$, supplemented with the one-point correlation function condition $c\widehat{f}(p=0) = \omega(a^*(f)) = 0$ or $c = 0$.

Next we derive an other general and useful property holding for arbitrary homogeneous states which can be quasi-free or not quasi-free. We show that for any translation invariant state ω with two-point functions determined by the operators (R,S), there exists always a canonical transformation τ mapping the state into a new state which has gauge invariant two-point functions, and is therefore determined by two operators of the type $(\widetilde{R},0)$. We determine explicitly the operator $\widetilde{R}$ as a function of the originally given state operators R and S.

This result is a generalization of a more restricted result stated in [115], where such a map is proved to exist within the set of generalized pure qf-states. Not only the existence but also the explicit construction and form of this canonical transformation τ for any initially given state ω is derived.

Lemma 2.6. *Let ω be any space invariant or homogeneous state with two-point truncated functions functions $r \geq 1$ and $t \geq 0$. Then there exists a canonical transformation τ mapping the given state into a new homogeneous state $\omega \circ \tau$ with two-point truncated correlation functions given by the pair of operators $(\widetilde{R}, \widetilde{S} = 0)$. If $\widetilde{r}(p)$ is the multiplication function of the operator $\widetilde{R}$ then it is given as a function of the original pair of functions (r,t) by the formula*

$$\widetilde{r} = \frac{1}{2} + (t^2 + \frac{1}{4})^{\frac{1}{2}} \tag{2.29}$$

Applying this result to quasi-free states, all this means the following. Let $\omega_{(R,S)}$ be a space homogeneous qf-state, there exists a canonical transformation τ mapping the state into a gauge invariant one, i.e. $\omega_{(R,S)} \circ \tau = \omega_{(\widetilde{R},0)}$, where the multiplication operator $\widetilde{r}$ is given by the formula above.

Proof. If $s(p) = 0$ for p in some domain then $S = 0$ and nothing has to be proved in that domain. Therefore assume that $s(p) \neq 0$. First we apply a canonical gauge transformation such that $s(p) = |s(p)|$, i.e. we take the parameter λ in (2.28) equal to

$-\frac{1}{2}\arg s(p)$. Then one considers a second canonical transformation γ, in the physics literature called *Bogoliubov transformation* Eq. (7.3), mapping the creation and annihilation operators $a(p)^\#$ into new ones $\widetilde{a}(p)^\#$, given by

$$\widetilde{a(p)} = \gamma(a(p)) = u(p)a(p) - v(p)a^*(-p) \tag{2.30}$$

where u and v are real functions on $\mathbb{R}^d$ satisfying $u(-p) = u(p)$, $v(-p) = v(p)$ and $u(p)^2 - v(p)^2 = 1$. One checks that the new ones satisfy again the CCR-relations. Consider the two equations

$$\begin{aligned} \widetilde{r(p)} &= \omega_{(\widetilde{R},0)}(a(p)a^*(p)) = \omega_{(R,S)}(\gamma(a(p)a^*(p))) \\ 0 = \widetilde{s(p)} &= \omega_{(\widetilde{R},0)}(a(p)a(-p)) = \omega_{(R,S)}(\gamma(a(p)a(-p))) \end{aligned}$$

in order to express $\widetilde{r(p)}$ as a function of $r(p)$ and $s(p)$ or preferably $t(p)$. One computes explicitly the following equations from the former ones, using the symmetry of $r(p)$ and $s(p)$.

$$\begin{aligned} \widetilde{r(p)} &= u(p)^2 r(p) + v(p)^2(r(p)-1) - 2u(p)v(p)s(p) \\ 0 &= u(p)^2 s(p) - u(p)v(p)(2r(p)-1) + v(p)^2 s(p) \end{aligned}$$

Looking at the second equation, one gets a quadratic equation for the function variable $x \equiv u/v$, which always takes values larger than 1 and therefore leading to a unique solution given by

$$x = \frac{r - \frac{1}{2} + \sqrt{(r-\frac{1}{2})^2 - s^2}}{s}$$

Using the relation between the functions s and t, namely $t^2 = r(r-1) - s^2$, one gets the function x expressed in the variables r, t:

$$x = \frac{r - \frac{1}{2} + \sqrt{t^2 + \frac{1}{4}}}{\sqrt{r(r-1) - t^2}}$$

Substitute this solution for x in the expressions for u and v:

$$u = \frac{x}{\sqrt{x^2-1}}, v = \frac{1}{\sqrt{x^2-1}}$$

Finally substitute this result in the first equation in order to obtain $\widetilde{r}$ as a function of r and t as expressed in the Lemma.

The canonical transformation τ of the Lemma is of course given by the composition of the gauge transformation used above with the Bogoliubov transformation. This proves the first part of the Lemma. Concerning the application to the quasi-free state case, the canonical transformation τ has to be composed with the appropriate field translation canonical transformation in order to get in due case a vanishing one-point function for the new state.

Some generalities related to the physics of ergodic boson states

After the above analysis about the structure of the set of general boson states as well as about its subset of quasi-free states, we recollect here the essentials about the correlation functions for an arbitrary ergodic state as defined above, see Eq. (2.12). We add some general and important physical interpretations. All this is with an eye kept on future applications.

First we consider the one and two-point correlation functions. The general two-point truncated correlation functions are given by the formulae

$$\omega(a(f)a^*(g))_t = \omega(a(f)a^*(g)) - \omega(a(f))\omega(a^*(g)) = \int dk\, \overline{f(k)}g(k)(r(k)-1)$$
$$\omega(a(f)a(g))_t = \omega(a(f)a(g)) - \omega(a(f))\omega(a(g)) = \int dk\, \overline{f(k)g(k)}s(k)$$

and the most general one-point function by

$$\omega(a^*(f)) = \hat{f}(0)\bar{c},\ \omega(a(f)) = \overline{\hat{f}}(0)c.$$

The translation invariance implies indeed

$$\omega(a^*(f)) = \int_\Lambda dx\, f(x)\omega(a^*(x)) = \int_V dx\, f(x)\omega(a^*(x=0)). \tag{2.31}$$

Hence, $\bar{c} = \omega(a^*(x=0))$. Moreover the constant c gets the following interpretation in the thermodynamic limit.

$$\bar{c} = \lim_V \omega\left(\frac{1}{V}\int_\Lambda dx\, a^*(x)\right)$$

and the ergodicity property of the state yields the equality

$$\rho_0 := \lim_V \omega\left(\frac{1}{V}a_0^* a_0\right) = \lim_V \omega\left(\frac{1}{V}\int_V dx\, a^*(x)\int_V dx\, a(x)\right) = |c|^2 \tag{2.32}$$

It is important to realize that this equality does not hold if the state is not ergodic.

Formula Eq. (2.32) can also be written in the form

$$\rho_0 - \lim_V |\omega(\frac{a_0}{\sqrt{V}})|^2 = 0$$

or more explicitly as follows

$$\lim_V \frac{1}{V^2}\int_{V\times V} dx\,dy\,\{\omega(a^*(x)a(x+y)) - \omega(a^*(x))\omega(a(x+y))\} = 0 \tag{2.33}$$

If $\rho_0 = 0$, then $c = 0$ or all terms vanish. However, if $\rho_0 > 0$, then also $c = \lim_V \omega(\frac{a_0}{\sqrt{V}}) = \omega(a(0)) \neq 0$, which means that the state can not be gauge invariant. The equation (2.33) expresses the property of the boson state ω of *showing off-diagonal long range order* [129].

The reader realizes that these explicit formulae, together with their interpretations, hold for the one- and two-point functions of any ergodic boson state independent of the fact that it is quasi-free or not quasi-free. Also the physical interpretations following below remain generally valid. These formulae hold for all homogeneous states of all homogeneous boson systems.

In particular one has the following physical picture. Looking at the definition formula of ρ_0, it is clear that it has to interpreted as the *zero-mode* or $(k=0)$-*density of particles* of the state ω. In particular, if for some boson system one can show that a ground or equilibrium state ω has the property $\rho_0 > 0$, then one can say that the state shows a macroscopic occupation of particles in the zero-mode. For such a state, the number of particles in the zero mode in a finite volume V has to increase proportionally with the volume (see Eq. (2.32)). Hence if

$$\rho_0 = \lim_V \frac{\omega(a_0^* a_0)}{V} > 0$$

one speaks about the occurrence of *Bose-Einstein condensation*, in short denoted by BEC, in that state and for the zero-mode. The value of ρ_0 itself is called the zero-mode *condensate density*.

Since by definition $\rho = \lim_V \omega(N_V/V)$, this quantity is called the *total density of particles* for the state ω. Since for all homogeneous states trivially holds that $\omega(a_k) = 0$ if $k \neq 0$, and because of Eq. (2.33) one gets for each ergodic state for which the thermodynamic limit($V \to \infty$) exists the formula

$$\omega(\frac{N_V}{V}) = \frac{1}{V}\sum_k \omega(a_k^* a_k) - \frac{1}{V}\omega(a_0^* a_0) + \frac{1}{V}\omega(a_0^* a_0) = \omega(\frac{N_V}{V})_t + \frac{1}{V}\omega(a_0^* a_0)$$

One obtains for all ergodic states for which the total density ρ is finite, the following universal relation:

$$\rho = \rho_0 + \rho_c \tag{2.34}$$

It expresses that the total density for the state is the sum of the zero-mode *condensate density* ρ_0 and the density ρ_c of all excited $(k \neq 0)$ particles. The latter one is called the *critical density*, in the case that there is a non-trivial condensate $(\rho_0 > 0)$. The critical density is explicitly given in terms of the two-point operator $r(p)$ by the formula

$$\rho_c = \int dk\,(r(k) - 1) \tag{2.35}$$

In general the density relation Eq. (2.34) is of vital importance in the study of Bose-Einstein condensation for solvable as well as for non-solvable fully interacting boson models.

Sofar we considered only the one and two-point functions of an ergodic state. As is clear from the general definition Eq. (2.12), in order to fix a state completely one has to know all truncated n-point functions for all n=1,2,3,.... It is always important to keep in mind that they should satisfy the necessary and sufficient positivity conditions implied by the positivity of the state. We do not enter into an explicit discussion about these positivity properties. It is a straightforward but a technically annoying matter to write these properties out in their explicit form in terms of the correlation functions. We just repeat the remark that the ergodicity of the state implies that the higher order truncated n-point functions with $n > 2$, can be described, exactly as we did with the two-point functions, by multiplication operators in n-1 variables, and that this approach is useful.

In the case of open boson systems, condensation in excited modes can also occur. This means that one has the possibility of macroscopic occupation of a non-zero mode, say $q \neq 0$, for some state ω. This is expressed by the formula:

$$\rho_q = \lim_V \frac{\omega(a_q^* a_q)}{V} > 0$$

describing a macroscopic occupation of the q-mode. One speaks of the occurrence of *q-condensation*, which is a fair form of Bose-Einstein condensation. In Chapter Eq. (4) we discuss a simple model showing q-condensation.

So far we considered only the situation of fully space translation invariant states, i.e. states invariant for the full space translation group $\mathbb{R}^d$. However the situation of the space translation invariance with respect to a sublattice G of $\mathbb{R}^d$ is also relevant as will become clear in the applications below. In that case, consider a state ω which is invariant under the translation group $G = |a|\mathbb{Z} \times \mathbb{R}^{d-1}$, i.e. the continuous translations in $d-1$ directions and the periodic lattice translations in one direction given by a vector of the form $a = |a|e$. It has a period of length $|a|$ and a direction along the unit vector e and it defines a corresponding momentum variable $q = e(2\pi/|a|)$. For each $x \in \mathbb{R}^d$ one can write $x = (ye, x_\perp)$, where $x_\perp$ is the x-component orthogonal to e and ye the e-component. For any such a G-invariant state $\widetilde{\omega}$ it could be meaningful to talk about the *q-condensate density* $\rho_q = \lim_V \widetilde{\omega}(\frac{a_q^* a_q}{V})$. Remark that one gets a full homogeneous state ω by integration over the period which is given by, for any observable X,

$$\omega(X) = \frac{1}{|a|} \int_0^{|a|} dy\, \widetilde{\omega} \circ \tau_y(X) \tag{2.36}$$

and a q-condensate density of the form

$$\rho_q = \lim_V \omega(\frac{a_q^* a_q}{V}) = \frac{1}{|a|} \int_0^{|a|} dy\, \widetilde{\omega}(a^*(y,0)a(y,0)) \tag{2.37}$$

Of course this construction extends to more dimensions up to all space directions.

All these definitions and physical interpretations about the one and two-point functions are of central importance in the language of physicists talking about fully interacting, respectively non-interacting boson systems studied with all the common techniques and concepts in many-body boson systems used since decades [81, 13, 79, 80]. As such they will remain of prime relevance in the rest of this monograph and in the future.

Springer

http://www.springer.com/978-0-85729-108-0

Many-Body Boson Systems
Half a Century Later
Verbeure, A.F.
2011, X, 190 p., Hardcover
ISBN: 978-0-85729-108-0