Local states of free bose fields

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1 Introduction

These notes contain an extended version of lectures given at the "Summer School on Large Coulomb Systems" in Nordfjordeid, Norway, in august 2003. They furnish a short introduction to some of the most basic aspects of the theory of quantum systems that have a dynamics generated by an equation of the form

$$\ddot{q} = -\Omega^2 q$$

where Ω is a self-adjoint, positive, invertible operator on a dense domain $\mathcal{D}(\Omega)$ in a real Hilbert space $\mathcal{K}$.

Such systems are usually referred to as free bose fields. They are really just harmonic systems and I will occasionally use the term oscillator fields since I will also discuss their *classical* counterparts and because I want to stress the instructive analogy with finite systems of coupled oscillators, which is very helpful when one tries to understand the underlying physical interpretation of the theory.

Many of the simplest systems of classical and quantum mechanics obey an equation of this form. Examples include (see Sect. 2.2):

(i) Finite dimensional systems of coupled oscillators, where $\mathcal{K} = \mathbb{R}^n$ and Ω is a positive definite matrix.

(ii) Lattices or chains of coupled oscillators, where $\mathcal{K} = \ell^2(\mathbb{Z}^d, \mathbb{R})$ and Ω is usually a bounded operator with a possibly unbounded inverse. Those are used to model lattice vibrations in solid state physics.

(iii) The wave equation, where $\mathcal{K} = L^2(K, \mathbb{R})$, $K \subset \mathbb{R}^d$ and $\Omega^2 = -\Delta$ with suitable boundary conditions.

(iv) The massive or massless Klein-Gordon equation on static spacetimes. These are a popular paradigm for studying quantum field theory on curved spacetimes.

Despite their supposed simplicity, these systems are interesting for at least two reasons. First, they provide examples where the basic concepts and meth-

ods of quantum field theory can be explained, understood and tested. Second, they provide the building blocks for the study of more complicated systems in quantum field theory and (non-equilibrium) statistical mechanics, where one or more such fields are (nonlinearly) coupled to each other or to other, possibly finite dimensional systems. Bose fields are for example a popular tool for modelling heath baths. The much studied spin-bose model and more generally the Pauli-Fierz models are all of this type.

In Section 2, I shall first briefly describe the classical mechanics of such systems in a unified way. This will then allow us in Section 3 to write down the corresponding quantum mechanical systems – the free bose fields – in a straightforward manner, for *both infinite and finite dimensional* systems. In particular, if you are familiar with the quantum mechanical description of finite dimensional systems, you should conclude after reading these two sections that the description of the infinite dimensional systems can be done quite analogously.

At that point, we will be ready to start studying the systems constructed, and to analyze their physical properties. The only issue I will address here, in Section 4, is not one that features prominently in quantum field theory books, but it has generated a fair amount of debate and even controversy. It is the one of local observables, and of local states, essential for the physical interpretation of the theory. Other topics will be discussed in [DB2]. I will adopt the definition of Knight of "strictly local excitation of the vacuum" (Definition 4), that I will refer to as a strictly local or a strictly localized state for brevity. I will then state and prove a generalization of Knight's Theorem [Kn] (Sect. 4.5) which asserts that finite particle states cannot be perfectly localized. It will furthermore be explained how Knight's a priori counterintuitive result can be readily understood if one remembers the analogy between finite and infinite dimensional harmonic systems alluded to above. I will also discuss the link between the above result and the so-called Newton-Wigner position operator thereby illuminating, I believe, the difficulties associated with the latter (Sect. 4.7). I will in particular argue that those difficulties do not find their origin in special relativity or in any form of causality violation, as is usually claimed. It will indeed be seen that the Newton-Wigner position operator has an immediate analog for a finite or infinite system of oscillators, and that it makes absolutely no sense there since it is at odds with basic physical intuition and since it is not compatible with the physically reasonable definition of Knight. The conclusion I will draw is that *the Newton-Wigner operator does not provide an appropriate tool to describe the strict localization properties of the states of extended systems of the type discussed here*. It shows up only because of an understandable but ill-fated desire to force too stringent a *particle interpretation* with all its usual attributes on the states of a *field*. The right notion of a (strictly) localized state is the one given by Knight. These issues have generated some debate in the context of relativistic quantum field theory over the years, upon which I shall comment in Sect. 4.7.

The text is written at the graduate level and is aimed at an audience of mathematicians with a taste for physics and of physicists with a taste for mathematics. A background in the classical and quantum theory of *finite* dimensional systems is assumed, although the text is basically self-contained. The approach to the subject chosen here differs both from the usual "second quantization" and "canonical quantization" treatments of quantum field theory prevalent in the physics literature (although it is very close to the latter). It is not axiomatic either. I feel it is fruitful because it allows one to apply the intuition gained from the study of finite dimensional systems in the infinite dimensional case. This helps in developing a good understanding of the basic physics of quantum field theory, and in particular to do away with some of the confusion surrounding even some of the simplest aspects of this theory, as I hope to illustrate with the discussion of "localization" in this context. Although my approach here is resolutely non-relativistic, I hope to show it still sheds an interesting and illuminating light on relativistic theories as well. Indeed, the main feature of the systems under consideration is their infinite spatial extension, and it is this feature that distinguishes them from systems with a finite number of particles such as atomic or molecular systems, that have a finite spatial extension.

Related topics will be discussed in a much extended version of this manuscript, which is in preparation [DB2].

2 Classical free harmonic systems

2.1 The Hamiltonian structure

Let us now turn to the systems described briefly in the Preface. My first goal is to describe in detail the Hamiltonian structure underlying

$$\ddot{q} + \Omega^2 q = 0. \tag{1}$$

For finite dimensional systems, it is well known how to view (1) as a Hamiltonian system, and we will now show how to do this for infinite dimensional systems using as only ingredient the positive operator Ω^2 on $\mathcal{D}(\Omega^2) \subset \mathcal{K}$. We need to identify a phase space on which the solutions to this equation define a Hamiltonian flow for a suitable Hamiltonian. For that purpose, note that, formally at least, (1) is equivalent to

$$\dot{q} = p, \ \dot{p} = -\Omega^2 q,$$

which are Hamilton's equations of motion for the Hamiltonian ($X = (q, p)$)

$$H(X) = \frac{1}{2} p \cdot p + \frac{1}{2} q \cdot \Omega^2 q, \tag{2}$$

with respect to the symplectic structure

$$s(X, X') = q \cdot p' - q' \cdot p.$$

Note that I use $\cdot$ for the inner product on $\mathcal{K}$. The Poisson bracket of two functions f and g on $\mathcal{K} \oplus \mathcal{K}$ is neatly expressed in terms of s by

$$\{f, g\} = s(\nabla_X f, \nabla_X g),$$

where $\nabla_X f = (\nabla_q f, \nabla_p f)$. Solving Hamilton's equations of motion one obtains the Hamiltonian flow which in this case can simply be written

$$\Phi_t = \cos \Omega t I_2 - \sin \Omega t J, \tag{3}$$

where

$$I_2 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad J = \begin{pmatrix} 0 & -\Omega^{-1} \\ \Omega & 0 \end{pmatrix}. \tag{4}$$

For later purposes, we remark that the corresponding Hamiltonian vector field X_H defined by

$$\frac{\mathrm{d}\Phi_t}{\mathrm{d}t} = X_H \Phi_t. \tag{5}$$

can be written

$$X_H = -J\Omega. \tag{6}$$

Of course, this is sloppy, because whereas s defines a symplectic structure on $\mathcal{K} \oplus \mathcal{K}$, the operator J is not a bounded operator on $\mathcal{K} \oplus \mathcal{K}$, so that the flow is not globally defined on this space! In other words, in the infinite dimensional case, we have to remember that both Ω and Ω^{-1} may be unbounded operators (think of the wave equation, for example) and therefore we have to carefully identify a suitable phase space on which both the symplectic structure and the flow Φ_t are globally well-defined. For that purpose, we introduce the scale of spaces ($\lambda \in \mathbb{R}$):

$$\mathcal{K}_\lambda = [\mathcal{D}(\Omega^\lambda)].$$

Here the notation [ ] means that we completed $\mathcal{D}$ in the topology induced by $\| \Omega^\lambda q \|$ where $\| \cdot \|$ is the Hilbert space norm of $\mathcal{K}$: note that we have supposed that Ω has a trivial kernel, so that $\| \Omega^\lambda q \|$ defines a norm (and not just a semi-norm). Explicit examples are developed in Sect. 2.2.

It is easy to check that J and hence Φ_t are globally well defined on

$$\mathcal{H} = \mathcal{K}_{1/2} \oplus \mathcal{K}_{-1/2}.$$

Moreover, the symplectic form can also defined on this space via

$$s(X, X') = \Omega^{1/2} q \cdot \Omega^{-1/2} p' - \Omega^{1/2} q' \cdot \Omega^{-1/2} p. \tag{7}$$

Actually, it can be checked that $\mathcal{H}$ is the only space of the form $\mathcal{K}_\lambda \oplus \mathcal{K}_\mu$ with these properties. In what follows, I shall refer to $\mathcal{H}$ as the (real) phase space of the system. Note that, from now on, whenever $w \in \mathcal{K}_\lambda, w' \in \mathcal{K}_{-\lambda}$, we will

write $w \cdot w' = \Omega^{\lambda} w \cdot \Omega^{-\lambda} w'$. With these notations, one easily checks that, for $a \in \mathcal{K}_{1/2}, b \in \mathcal{K}_{-1/2}$,

$$\{b \cdot q, a \cdot p\} = a \cdot b. \tag{8}$$

Here $\{\cdot, \cdot\}$ denotes the Poisson bracket.

Note that the phase space $\mathcal{H}$ may depend on Ω, for fixed $\mathcal{K}$. As long as both Ω and Ω^{-1} are bounded operators, one has clearly $\mathcal{H}(\Omega) = \mathcal{K} \oplus \mathcal{K}$. This is of course always the case when $\mathcal{K}$ is finite dimensional. So for systems with a finite number of degrees of freedom, the phase space is fixed a priori to be $\mathcal{K} \oplus \mathcal{K}$, and the dynamics can be defined a posteriori on this fixed phase space. However, whenever either Ω or Ω^{-1} are unbounded, $\mathcal{H}(\Omega)$ differs from $\mathcal{K} \oplus \mathcal{K}$ and depends explicitly on Ω. In other words, one cannot first choose the phase space, and then study various different dynamics on it. Instead, the phase space and the dynamics are intimately linked: changing the dynamics on a given fixed phase space may not make sense.

To conclude, so far, we have shown how the solutions of (1) define a (linear) Hamiltonian flow Φ_t on a (real) symplectic vector space $(\mathcal{H}, s)$.

As far as the classical mechanics of the system is concerned, this is really all we need. In order to construct the corresponding quantum theory (Section 3), and in particular the quantum Hilbert space, we do however need to exploit the structures underlying the classical theory some more. This I will do in Sect. 2.3. If we were only interested in the finite dimensional case, this would be of some interest, but not necessary. For the infinite dimensional case it is essential. Indeed, for finite dimensional harmonic systems, the usual Schrödinger quantum mechanics is of course perfectly adequate, and the formalism developed here is quite useless. It is however not possible to straightforwardly adapt the Schrödinger formulation to the infinite dimensional situation, and so we need to exploit the additional structures a little more. To understand the following developments, it is helpful to have some examples in mind.

2.2 Examples

Coupled oscillators: finite dimension

Systems of point masses connected by springs have Hamiltonians of the type

$$H(X) = \frac{1}{2}(p^2 + q \cdot \Omega^2 q)$$

where $X = (q, p) \in \mathbb{R}^{2n}$, so that here $\mathcal{K} = \mathbb{R}^n$, and Ω^2 is a positive definite $n \times n$ matrix. More generally, this Hamiltonian arises when linearizing any potential about a stable equilibrium point. An instructive example is the finite *oscillator chain* with periodic boundary conditions (see Fig. 1). There, n particles, constrained to move in one dimension only, are placed on a ring. They interact with their nearest neighbours only, through a force that is linear in the relative displacement of the particles and that is characterized by

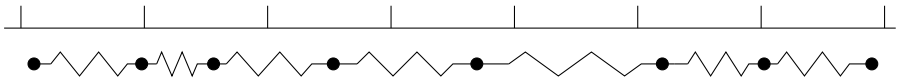

Fig. 1. A schematic representation of a chain of 8 oscillators moving horizontally. Linking the first to the last, you get a ring. The tick marks indicate their equilibrium positions. In the figure $\omega_{\rm w} = 0$.

a frequency $\omega_{\rm n}$. In addition they are each subjected to a harmonic force with frequency $\omega_{\rm w}$. Assuming all the particles have identical masses, set equal to 1, the Hamiltonian for this system reads

$$H(X) = \frac{1}{2}\left(\sum_{i=1}^{n}(p(i)^2 + \omega_{\rm w}^2 q(i)^2 + \omega_{\rm n}^2(q(i+1) - q(i))^2\right).$$

Note that in the sum the index is to be taken periodically, so that $q(n+1) = q(1)$, *etc.*. I have adopted here and will continue to use the somewhat unusual notation $v(i)$ for the ith component of a vector $v \in \mathbb{R}^n$ or $\mathbb{C}^n$. This will prove very convenient later on. Introducing $\omega_0^2 = \omega_{\rm w}^2 + 2\omega_{\rm n}^2 > 0$ and

$$0 \leq \nu = \frac{\omega_{\rm n}^2}{\omega_0^2} \leq 1/2,$$

the equation of motion is, for all $j = 1, \ldots n$,

$$\ddot{q}(j) = -\omega_0^2\left[q(j) - \nu(q(j+1) + q(j-1))\right] = -(\Omega^2 q)(j). \tag{9}$$

One readily finds the eigenvalues of Ω^2: they are given by

$$\omega^2(k) = \omega_0^2[1 - 2\nu\cos 2\pi k] \quad k = 1/n, 2/n, \ldots 1.$$

Note that the eigenvalues are indeed positive, but, in order to make sure that 0 is not an eigenvalue, we have to impose $\nu < 1/2$, which amounts to requiring that $\omega_{\rm w} \neq 0$. This is intuitively clear: if $\omega_{\rm w} = 0$, the system allows for stationary solutions in which all oscillators are displaced by the same amount, so that the springs between the oscillators are not stretched. These are are referred to as a "zero modes". The above Hamiltonian provides the simplest model possible for a harmonic crystal, and is discussed in all books on solid state physics both from the classical and the quantum mechanical point of view.

Oscillator chains and lattices

Having understood the finite oscillator chain, it is easy to understand the first infinite dimensional system we shall consider, which is an infinite linear chain

of oscillators, each one linked to its neighbours and to a wall with identical springs, so that the system is translationally invariant. The Hamiltonian and equation of motion of this system are the same as in the case of the ring, except that the sums now run over $\mathbb{Z}$. We now have $\mathcal{K} = \ell^2(\mathbb{Z}, \mathbb{R})$ and Ω^2, defined precisely as in (9) is a bounded operator. It has a purely absolutely continuous spectrum $\{\omega^2(k) \mid k \in [0, 1]\}$, for all values of $\nu \in [0, 1/2]$. Indeed, even if $\nu = 1/2$, 0 is not an eigenvalue of Ω^2, since η_0 does not belong to $\ell^2(\mathbb{Z}, \mathbb{R})$.

It is instructive to identify the spaces $\mathcal{K}_\lambda$ explicitly in this case. For that purpose, note that the Fourier series transform

$$\hat{q}(k) = \sum_{j \in \mathbb{Z}} q(j) \mathrm{e}^{-\mathrm{i}2\pi jk}$$

identifies the real Hilbert space $\ell^2(\mathbb{Z}, \mathbb{R})$ with the real subspace of the complex Hilbert space $L^2(\mathbb{R}/\mathbb{Z}, dk, \mathbb{C})$ for which $\overline{\hat{q}(k)} = \hat{q}(-k)$. It follows that $\mathcal{K}_\lambda$ can be identified with the space of locally integrable functions $\hat{q}$ for which $\overline{\hat{q}(k)} = \hat{q}(-k)$ and, more importantly, $\omega(k)^\lambda \hat{q}(k)$ belongs to $L^2(\mathbb{R}/\mathbb{Z}, dk, \mathbb{C})$.

First of all, consider $0 \leq \nu < 1/2$. Then the spectrum is bounded away from zero, which means that both $\omega(k)$ and $\omega(k)^{-1}$ are bounded functions of k. As a result, then, for all $\lambda \in \mathbb{R}$, $\mathcal{K}_\lambda = \ell^2(\mathbb{Z}, \mathbb{R})$. In particular, then $\mathcal{H} = \ell^2(\mathbb{Z}, \mathbb{R}) \times \ell^2(\mathbb{Z}, \mathbb{R})$ and does *not* depend on the value of ν in the range considered.

Something interesting happens, however, if we consider the case $\nu = 1/2$. Remember that this corresponds to setting $\omega_\mathrm{w} = 0$, which was not allowed in the finite ring because of the existence of the zero mode. Some remnant of this problem shows up here. Indeed, consider $\mathcal{K}_\lambda$, for $\lambda < 0$. Since

$$\omega^2(k) = (2\pi\omega_0)^2 k^2 + \mathrm{o}(k^2),$$

$q \in \mathcal{K}_\lambda$ if and only if $|k|^\lambda \hat{q}(k)$ belongs to $L^2(\mathbb{R}/\mathbb{Z}, dk, \mathbb{C})$ (and of course satisfies $\overline{\hat{q}(k)} = \hat{q}(-k)$). But, for $\lambda = -1/2$, this is not true for all $q \in \ell^2(\mathbb{Z}, \mathbb{R})$. As a result, $\mathcal{K} = \ell^2(\mathbb{Z}, \mathbb{R})$ is not a subspace of $\mathcal{K}_{-1/2}$ and similarly $\mathcal{K}_{1/2}$ is not a subspace of $\mathcal{K} = \ell^2(\mathbb{Z}, \mathbb{R})$. Hence the phase space $\mathcal{H}$ is now different, as a set, from the phase space when $\nu \neq 1/2$ and in addition, one phase space is not included in the other. To see this has noticeable physical consequences, note the following. It seems like a reasonable thing to wish to study the motion of the chain when initially only one of the degrees of freedom is excited. Suppose therefore you wish to pick the initial condition $q(i) = p(i) = 0$, for all $i \neq 0$, $q(0) = 0 \neq p(0)$. In other words, the oscillator at the origin starts from its equilibrium position with a non-zero initial speed, while all other oscillators are at rest at their equilibrium positions. The trouble is that, when $\nu = 1/2$, this initial condition does not belong to the phase space! So it should be remembered that the choice of phase space I made here, which is reasonable from many a point of view, seems to nevertheless be somewhat too restrictive in this particular case, since it excludes certain very reasonable

initial conditions from the state space of the system. This is one aspect of the so-called infrared problem and it will be relevant when discussing local observables in Section 4.

The generalization of the preceding considerations to d-dimensional translationally invariant lattices of oscillators is immediate. One has $\mathcal{K} = \ell^2(\mathbb{Z}^d, \mathbb{R})$ and, for all $j \in \mathbb{Z}^d$,

$$(\Omega^2 q)(j) = \omega_{\rm w}^2 q(j) - \omega_{\rm n}^2 \sum_{i \in {\rm nn}(j)} (q(i) - q(j)) = \omega_0^2 q(j) - \omega_{\rm n}^2 \sum_{i \in {\rm nn}(j)} q(i), \quad (10)$$

where ${\rm nn}(j)$ designates the set of nearest neighbours of j and where this time

$$\omega_0^2 = \omega_{\rm w}^2 + 2d\omega_{\rm n}^2 \qquad \text{and} \qquad 0 \leq \nu = \frac{\omega_{\rm n}^2}{\omega_0^2} \leq \frac{1}{2d}.$$

Using the Fourier transform to diagonalize Ω^2 one finds the dispersion relation

$$\omega(k)^2 = \omega_0^2 \left[1 - 2\nu \left(\sum_{i=1}^{d} \cos 2\pi k_i \right) \right].$$

This time the critical value of ν is $1/2d$ but it leads to less severe infrared behaviour. Indeed, if $\nu = 1/2d$, then

$$\omega(k)^2 = \omega_0^2 \frac{1}{d} \sum_{i=1}^{d} (2\pi k_i)^2 + {\rm o}(|k|^2) = \frac{(2\pi\omega_0)^2}{d} |k|^2 + {\rm o}(|k|^2).$$

But now all compactly supported q belong to $\mathcal{K}_\lambda$, for all $-d/2 < \lambda$, as is easily checked. As a result, this time the phase space $\mathcal{H}$ contains all such initial conditions as soon as $d \geq 2$. We shall refer to them as *strictly local perturbations from equilibrium* and study their quantum analogues in Section 4. To be more precise, if $d \geq 2$, and if we denote by $C_{\rm c}(\mathbb{Z}^d)$ the space of compactly supported sequences, then $C_{\rm c}(\mathbb{Z}^d) \times C_{\rm c}(\mathbb{Z}^d) \subset \mathcal{H}$, for all possible values of ν. If $X = (q, p) \in C_{\rm c}(\mathbb{Z}^d) \times C_{\rm c}(\mathbb{Z}^d)$, then X describes an initial state in which only a finite number of oscillators is displaced from their equilibrium position and/or moving. So for this rather large and very natural class of initial conditions, the dynamics can be investigated as a function of ν, for all possible values of ν.

Lattices of oscillators are used to describe the thermal and acoustic properties of various solids, such as metals, crystals of all sorts, amorphous materials *etc.*. Putting $\omega_{\rm n} = 0$ in the expressions above, one obtains the so-called Einstein model, in which the oscillators representing the ions of the solid are not coupled. The case where $\omega_{\rm n} \neq 0$ is the Debye model. In more sophisticated models still, different geometries may appear (hexagonal lattices, body or face centered cubic lattices *etc.*), and the spring constants may vary from site to site in periodic, quasi-periodic or random ways.

Wave and Klein-Gordon equations

The wave equation

$$\partial_t^2 q(x,t) = \Delta q(x,t)$$

on a domain $K \subset \mathbb{R}^d$ with Dirichlet boundary conditions is another example of a free oscillator field where $\mathcal{K} = L^2(K,\mathbb{R})$ and $\mathcal{D}(\Omega)$ is the domain of the square root of the Dirichlet Laplacian. When K is a bounded set, the spectrum of the Dirichlet Laplacian is discrete. No infrared problem then arises, reflecting the fact that no arbitrary long wavelengths can occur in the system.

The case where $K = \mathbb{R}^d$ is instructive and easy to work out thanks to its translational invariance. The situation is completely analogous with the one in Sect. 2.2. Writing $\omega(k) = \sqrt{k^2}$, the space $\mathcal{K}_\lambda$ is for each real λ naturally isomorphic to the real subspace of $L^2(\mathbb{R}^d, \omega(k)^{2\lambda}dk, \mathbb{C})$ given by the condition $\overline{\hat{q}(k)} = q(-k)$. If $d \geq 2$, the Schwartz space is a subspace of $\mathcal{K}_{\pm\frac{1}{2}}$.

One can also consider the more general case where K is a Riemannian manifold with metric γ and $-\Delta$ the corresponding Laplace-Beltrami operator. Replacing $-\Delta$ by $-\Delta + m^2$ $(m > 0)$ in the above, one obtains the Klein-Gordon equation. It plays an important role in the relativistic quantum field theory on flat or curved spacetimes.

2.3 A preferred complex structure on the *real* classical phase space $\mathcal{H}$

The simple linear systems we are dealing with here have some extra structure that is encoded in the matrix J defined in (4). Noticing that $J^2 = -I_2$, one sees J defines an s-compatible (*i.e.* $s(JX, JY) = s(X,Y)$) and positive definite (*i.e.* $s(X, JX) \geq 0$ and $s(X, JY) = 0, \forall Y \in \mathcal{H}$ implies $X = 0$) complex structure on $\mathcal{H}$. As a result, $\mathcal{H}$ can first of all be viewed as a real Hilbert space, with inner product

$$g_\Omega(X,Y) \stackrel{\text{def}}{=} s(X, JY) = \sqrt{\Omega}q \cdot \sqrt{\Omega}q' + \sqrt{\Omega}^{-1}p \cdot \sqrt{\Omega}^{-1}p', \qquad (11)$$

where $Y = (q', p')$. Of course, we recognize here the natural inner product on $\mathcal{H} = \mathcal{K}_{1/2} \oplus \mathcal{K}_{-1/2}$, written in terms of the symplectic form and J.

In addition, J can be used to equip $\mathcal{H}$ with a *complex* Hilbert space structure, where multiplication with the complex number $a + \mathrm{i}b \in \mathbb{C}$ is defined by

$$(a + \mathrm{i}b)X \stackrel{\text{def}}{=} (a + bJ)X, \quad \forall X \in \mathcal{H}$$

and with the inner product

$$\langle X, Y\rangle_+ = \frac{1}{2}(g_\Omega(X,Y) + \mathrm{i}s(X,Y)). \qquad (12)$$

Note that, when $\mathcal{H}$ has $2n$ *real* dimensions, the complex vector space $(\mathcal{H}, J)$ has only n complex dimensions.

Since Φ_t is symplectic and commutes with J, one easily checks that

$$g_\Omega(\Phi_t X, \Phi_t Y) = g_\Omega(X, Y) \quad \text{and} \quad \langle \Phi_t X, \Phi_t Y \rangle_+ = \langle X, Y \rangle_+,$$

so that Φ_t is a unitary operator on the complex Hilbert space $(\mathcal{H}, J, \langle \cdot, \cdot \rangle_+)$. As a result, $X_H = -J\Omega$, the generating Hamiltonian vector field is necessarily anti-self-adjoint and one can check that in addition

$$\mathrm{i}\langle X, X_H X \rangle_+ = H(X). \tag{13}$$

It is natural to wonder if there exist many complex structures on $\mathcal{H}$ with these properties. In fact, J is the unique s-compatible, positive complex structure on $\mathcal{H}$ so that Φ_t is unitary on the corresponding complex Hilbert space [DB2]. In other words, the phase space $\mathcal{H}$ of an oscillator field, which is a *real* symplectic space, carries a natural, flow-invariant complex Hilbert space structure!

The ensuing complex Hilbert space seems a somewhat abstract object, but it can be naturally identified with $\mathcal{K}^{\mathbb{C}}$, the complexification of $\mathcal{K}$, as I now explain. In the following, whenever V is a real vector space, $V^{\mathbb{C}} = V \oplus \mathrm{i}V$ will denote its complexification. In the concrete examples I have in mind, where $V = \mathcal{K} = \mathbb{R}^n, \ell^2(\mathbb{Z}^d, \mathbb{R})$ or $L^2(\mathbb{R}^d, \mathbb{R})$, one finds $V^{\mathbb{C}} = \mathcal{K}^{\mathbb{C}} = \mathbb{C}^n, \ell^2(\mathbb{Z}^d, \mathbb{C})$ or $L^2(\mathbb{R}^d, \mathbb{C})$, respectively. The identification goes as follows :

$$z_\Omega : X = (q, p) \in \mathcal{H} \mapsto z_\Omega(X) = \frac{1}{\sqrt{2}}(\sqrt{\Omega} q + \mathrm{i}\frac{1}{\sqrt{\Omega}} p) \in \mathcal{K}^{\mathbb{C}}. \tag{14}$$

The following proposition is then easily proven.

Proposition 1. *The map z_Ω defines an isomorphism between the complex Hilbert spaces $(\mathcal{H}, J, \langle \cdot, \cdot \rangle_+)$ and $\mathcal{K}^{\mathbb{C}}$, intertwining the dynamics Φ_t with $\mathrm{e}^{-\mathrm{i}\Omega t}$. More precisely,*

$$z_\Omega(JX) = \mathrm{i} z_\Omega(X) \quad \overline{z_\Omega(X)} \cdot z_\Omega(X') = \langle X, X' \rangle_+. \tag{15}$$

and

$$z_\Omega(\Phi_t X) = \mathrm{e}^{-\mathrm{i}\Omega t} z_\Omega(X). \tag{16}$$

Note that $\cdot$ has been extended to $\mathcal{K}^{\mathbb{C}}$ by linearity in each variable so that the inner product on $\mathcal{K}^{\mathbb{C}}$ is given by $\bar{z} \cdot z'$, for $z, z' \in \mathcal{K}^{\mathbb{C}}$. The choice of the unnatural looking factor $1/\sqrt{2}$ in the definition of z_Ω and of the matching factor $1/2$ in $\langle X, X' \rangle_+$ are conventions chosen to make comparison to the physics literature simple, as we will see further on. Similarly, for later purposes, we define

$$z_\Omega^\dagger : X = (q, p) \in \mathcal{H} \mapsto z_\Omega^\dagger(X) = \frac{1}{\sqrt{2}}(\sqrt{\Omega} q - \mathrm{i}\frac{1}{\sqrt{\Omega}} p) \in \mathcal{K}^{\mathbb{C}}, \tag{17}$$

which is complex anti-linear

$$z^\dagger_\Omega(JX) = -\mathrm{i}z^\dagger_\Omega(X) \tag{18}$$

and

$$\overline{z^\dagger_\Omega(X)} \cdot z^\dagger_\Omega(X') = \overline{\langle X, X'\rangle_+}. \tag{19}$$

The linear map z_Ω is readily inverted and one has, in obvious notations

$$q = \frac{1}{\sqrt{2\Omega}}(z_\Omega(X) + z^\dagger_\Omega(X)) \text{ and } p = \frac{\sqrt{\Omega}}{\mathrm{i}\sqrt{2}}(z_\Omega(X) - z^\dagger_\Omega(X)), \tag{20}$$

and

$$H(X) = z_\Omega(X)^\dagger \cdot \Omega z_\Omega(X). \tag{21}$$

In conclusion, we established that, having started with a *real* Hilbert space $\mathcal{K}$ and a positive self-adjoint operator Ω, the classical phase space $\mathcal{H}$ of the corresponding oscillator equation $\ddot{q} = -\Omega^2 q$ can be identified naturally with the *complex* Hilbert space $\mathcal{K}^\mathbb{C}$, on which the dynamics is simply the unitary group generated by Ω, the symplectic structure is the imaginary part of the inner product and the Hamiltonian is given by $H(z) = \overline{z} \cdot \Omega z$. We therefore ended up with a *mathematically* completely equivalent description of the original phase space $\mathcal{H}$, its symplectic structure and the dynamics Φ_t generated by the Hamiltonian H in (2).

It is however important to understand that the *physical* interpretation of this new formulation should be done carefully, as I explain in Sect. 2.4.

2.4 Physical interpretation

It is instructive to first look at what the formalism of the Sect. 2.3 yields for *finite dimensional* systems of coupled oscillators, such as the oscillator ring. In that case $\mathcal{K} = \mathbb{R}^n$ and hence $\mathcal{K}^\mathbb{C} = \mathbb{C}^n$. Note however that the identification of $\mathbb{R}^{2n}$ with $\mathbb{C}^n$ depends in a non-trivial way on Ω which makes a direct interpretation of points of $\mathbb{C}^n$ difficult. In particular, let $X = (q, p) \in \mathbb{R}^{2n} = \mathcal{H}$. Then the components of q and p have a direct physical interpretation as the displacements and momenta of the different oscillators. The ith component of the corresponding vector $z = z_\Omega(X) \in \mathbb{C}^n$ does not have such a direct simple interpretation since it is not a function of the diplacement q_i and momentum p_i of the ith oscillator alone, but it is a function of the diplacements q_j and momenta p_j of all the oscillators. This is so because in general, the matrix $\Omega^{1/2}$ has no (or few) zero off-diagonal entries, even if Ω^2 is tri-diagonal, as in the oscillator chain. Indeed, in that case, Ω^2 is a difference operator, but $\Omega^{1/2}$ is not. Conversely, as is clear from (20), q_i and p_i depend on all components of $z_\Omega(X)$, not only on the ith one. This explains why the alternative formulation of the problem in terms of the complex space $\mathcal{K}^\mathbb{C} = \mathbb{C}^n$ is not found in classical mechanics textbooks. Indeed, one is typically interested in questions concerning the displacements of the different oscillators, the energy distribution over the oscillators when the system is in a normal mode, energy

propagation along the oscillators when originally only one oscillator is excited, *etc.*. Such questions are obviously more easily addressed in the original formulation.

Another way to see why the alternative formulation leads to interpretational problems is as follows. Suppose we are studying two oscillator systems, one with potential $\frac{1}{2}q \cdot \Omega^2 q$ and another with $\frac{1}{2}q \cdot \Omega'^2 q$, where $\Omega^2 \neq \Omega'^2$. To fix ideas, we can think of Ω'^2 as being a perturbation of Ω^2 which is obtained by changing just one spring constant. Suppose now that the state of the first system is $z \in \mathcal{K}^{\mathbb{C}}$, and of the second is $z' \in \mathcal{K}^{\mathbb{C}}$. Suppose $z = z' = z_0 \in \mathbb{C}^n$. Would you say the two systems are in the same state? Certainly not in general! Indeed, as a result of what precedes, and in particular of (20), the same point $z_0 \in \mathcal{K}^{\mathbb{C}}$ yields entirely different values for the displacements q_i, q_i' and the momenta p_i, p_i' of the two oscillator systems! Indeed, we would normally say that the two systems are in the same state if the positions q_i, q_i' and momenta p_i, p_i' of the different degrees of freedom take the same values, that is to say if $X = X'$. But that is not the same as saying $z = z'$. In other words, if you decide to say $\mathcal{K}^{\mathbb{C}}$ is the phase space of your system, you should always remember that the physical interpretation of its points *depends on the dynamics, i.e.* on Ω. A similar phenomenon produces itself in the quantum mechanical description of oscillator systems as we will see in Sect. 3.3.

Suppose now we deal with an infinite dimensional oscillator field, such as an oscillator chain or a wave equation. As in the finite dimensional case, the elements of $\mathcal{H}$ then have a direct interpretation in terms of oscillator displacements, wave propagation *etc.*, whereas those of $\mathcal{K}^{\mathbb{C}}$ don't. But now an additional complicating phenomenon that we already pointed out occurs: starting with a fixed $\mathcal{K}$, different choices of Ω may lead to different phase spaces $\mathcal{H}$! We gave an example for the oscillator chain in Sect. 2.2. Talking about "the same state" for different systems now becomes very difficult, since the state space $\mathcal{H}$ depends on the system considered. It is then tempting to prefer the alternative formulation where the phase space $\mathcal{K}^{\mathbb{C}}$ is independent of the dynamics, but at that point it should always be remembered that the same point in $\mathcal{K}^{\mathbb{C}}$ has a different interpretation depending on which system you consider.

In spite of those interpretational difficulties, the alternative formulation of the classical mechanics of oscillator systems will turn out to be useful (and even crucial) in the quantum mechanical description of oscillator fields. Indeed, the quantum Hilbert space for the free oscillator field will be seen to be the symmetric Fock space over $(\mathcal{H}, J, \langle\cdot,\cdot\rangle_+)$ (see Section 3). But identifying the latter with $\mathcal{K}^{\mathbb{C}}$ allows one to conveniently identify the quantum Hilbert space as the symmetric Fock space over $\mathcal{K}^{\mathbb{C}}$. This way, one can work on a fixed Hilbert space, while changing the dynamics by perturbing Ω, for example. This is very convenient. Still, the rather obvious, seemingly trivial and innocuous remarks above concerning the interpretation of the *classical* field theory are at the origin of further, more subtle interpretational difficulties

with the quantum field theory of infinite dimensional oscillator fields as well, to which I shall come back in Sects. 3.3 and 3.5.

2.5 Creation and annihilation functions on $\mathcal{H}$

For the purposes of quantum mechanics, it will turn out to be convenient to develop the previous considerations somewhat further. Everybody is familiar with creation and annihilation operators in quantum mechanics. These objects are usually described as typically quantum mechanical in nature, but they have a perfectly natural classical analog, that I will call the creation and annihilation functions, and that are defined as follows.

For all $\xi \in \mathcal{K}^{\mathbb{C}}$,

$$a_{\mathrm{c}}(\xi) : X \in \mathcal{H} \mapsto \bar{\xi} \cdot z_{\Omega}(X) \in \mathbb{C},$$

and

$$a_{\mathrm{c}}^{\dagger}(\xi) : X \in \mathcal{H} \mapsto \xi \cdot z_{\Omega}^{\dagger}(X) \in \mathbb{C}.$$

Note that $a_{\mathrm{c}}(\xi)$ is anti-linear in ξ, whereas $a_{\mathrm{c}}^{\dagger}(\xi)$ is linear. The index "c" stands for "classical", so that the notation distinguishes between the classical creation/annihilation functions and the quantum creation/annihilation operators, to be introduced later. A direct computation now yields

$$\{a_{\mathrm{c}}(\xi_1), a_{\mathrm{c}}^{\dagger}(\xi_2)\} = -\mathrm{i}\bar{\xi}_1 \cdot \xi_2$$

and

$$a_{\mathrm{c}}(\xi) \circ \Phi_t = a_{\mathrm{c}}(\mathrm{e}^{\mathrm{i}\Omega t}\xi), \quad a_{\mathrm{c}}^{\dagger}(\xi) \circ \Phi_t = a_{\mathrm{c}}^{\dagger}(\mathrm{e}^{\mathrm{i}\Omega t}\xi).$$

Also, for all $\eta \in \mathcal{K}^{\mathbb{C}}_{-1/2}$

$$\eta \cdot q = \frac{1}{\sqrt{2}}(a_{\mathrm{c}}(\Omega^{-1/2}\bar{\eta}) + a_{\mathrm{c}}^{\dagger}(\Omega^{-1/2}\eta)) = \frac{-\mathrm{i}}{\sqrt{2}}(a_{\mathrm{c}}^{\dagger}(\mathrm{i}\Omega^{-1/2}\eta) - a_{\mathrm{c}}(\mathrm{i}\Omega^{-1/2}\bar{\eta})), \tag{22}$$

and, similarly, for all $\eta \in \mathcal{K}^{\mathbb{C}}_{1/2}$

$$\eta \cdot p = \frac{\mathrm{i}}{\sqrt{2}}(a_{\mathrm{c}}^{\dagger}(\Omega^{1/2}\eta) - a_{\mathrm{c}}(\Omega^{1/2}\bar{\eta})). \tag{23}$$

In the language of the physics literature, these two equations express the oscilator field $\eta \cdot q$ and its conjugate field $\eta \cdot p$ *viewed as functions on phase space* in terms of the creation and annihilation functions.

It is finally instructive to write H explicitly in terms of the annihilation and creation functions. This is easily done when Ω has pure point spectrum, *i.e.* when there exists a basis of normalized eigenvectors for Ω on $\mathcal{K}^{\mathbb{C}}$:

$$\Omega\eta_i = \omega_i\eta_i, \ i \in \mathbb{N}.$$

Then, from (21)

$$H = \frac{1}{2}\sum_i \omega_i \left(a_{\rm c}^\dagger(\eta_i)a_{\rm c}(\eta_i) + a_{\rm c}(\bar\eta_i)a_{\rm c}^\dagger(\bar\eta_i)\right). \tag{24}$$

Note that both sides of this equation are functions on (a suitable subset of) $\mathcal{H}$. Correspondingly, in quantum mechanics, both sides will be operators on the quantum Hilbert space of states.

3 The quantum theory of free harmonic systems

3.1 Finite dimensional harmonic systems: the Schrödinger representation

How to give a quantum mechanical description of the classical free oscillator fields studied in Section 2? I shall proceed in two steps. I will first recall the quantum description of a system of a finite number of coupled oscillators, and then rewrite it in a manner suitable for immediate adaptation to infinite dimension.

The quantum Hamiltonian for a system with n degrees of freedom having a classical Hamiltonian given by

$$H = \frac{1}{2}p^2 + V(q),$$

where the potential V is a (smooth) real-valued function on $\mathbb{R}^n$ is, in the so-called position (or Schrödinger) representation given by

$$H = \frac{1}{2}P^2 + V(Q),$$

where $P = -\mathrm{i}\partial/\partial x$ and $Q = x$ are the usual momentum and position operators which are self-adjoint on there natural domains in the "quantum state space" $L^2(\mathbb{R}^n, \mathrm{d}x)$. Note that, just as in the classical description, the state space is independent of the dynamics, which makes it easy to compare the dynamics generated by two different Hamiltonians H and H', with potentials V and V'. To put it differently, just as a given point X in the classical phase space $\mathbb{R}^{2n}$ corresponds to the same state of the system, whatever its dynamics, so a given ψ in $L^2(\mathbb{R}^n)$ yields the same position and momentum distributions for the system, whatever the dynamics to which it is subjected.

Consequently, for an n-dimensional system of coupled oscillators with classical configuration space $\mathcal{K} = \mathbb{R}^n$ and phase space $\mathcal{H} = \mathbb{R}^{2n}$ the quantum Hamiltonian reads

$$H = \frac{1}{2}(P^2 + Q\cdot\Omega^2 Q).$$

Unfortunately, these expressions stop making sense when $\mathcal{K}$ is an infinite dimensional space, in particular since it is not possible to make sense out of

$L^2(\mathcal{K})$ in that case. So to describe the quantum mechanics of infinite dimensional harmonic systems, I will first rewrite the above Hamiltonian differently, in a manner allowing for immediate generalization to infinite dimension. This rewriting is, as we shall see, very analogous to the rewriting of the classical mechanics on $\mathcal{K}^{\mathbb{C}} = \mathbb{C}^n$, explained in Sect. 2.3, and is therefore also affected by the interpretational difficulties mentioned in Sect. 2.4. It is nevertheless very efficient and essential.

Let's define, for any $\xi \in \mathcal{K}^{\mathbb{C}} = \mathbb{C}^n$, the so-called creation and annihilation operators

$$\tilde{a}(\xi) = \overline{\xi} \cdot \frac{1}{\sqrt{2}}(\Omega^{1/2}Q + \mathrm{i}\Omega^{-1/2}P), \quad \tilde{a}^\dagger(\xi) = \xi \cdot \frac{1}{\sqrt{2}}(\Omega^{1/2}Q - \mathrm{i}\Omega^{-1/2}P). \tag{25}$$

Note that those are first order differential operators, and that they depend on Ω, although the notation does not bring this dependence out. One checks easily that

$$\left[\tilde{a}(\xi), \tilde{a}^\dagger(\xi')\right] = \overline{\xi} \cdot \xi', \tag{26}$$

all other commutators vanishing. In addition, for any $\eta \in \mathbb{C}^n$,

$$\eta \cdot Q = \frac{1}{\sqrt{2}}(\tilde{a}(\Omega^{-1/2}\bar{\eta}) + \tilde{a}^\dagger(\Omega^{-1/2}\eta)), \tag{27}$$

and, similarly,

$$\eta \cdot P = \frac{\mathrm{i}}{\sqrt{2}}(\tilde{a}^\dagger(\Omega^{1/2}\eta) - \tilde{a}(\Omega^{1/2}\bar{\eta})). \tag{28}$$

The analogy of this and of the rest of this section with the developments of Sect. 2.5 should be self-evident. In particular, it is clear that the creation and annihilation operators are the "quantization" of the creation and annihilation functions $a_{\mathrm{c}}, a_{\mathrm{c}}^\dagger$ introduced earlier.

Furthermore, let $\eta_i \in \mathcal{K}^{\mathbb{C}} = \mathbb{C}^n, i = 1 \ldots n$ be an orthonormal basis of eigenvectors of Ω^2 with eigenvalues $\omega_1^2 \leq \omega_2^2 \leq \ldots \leq \omega_n^2$. Then it is easily checked that

$$H = \frac{1}{2}\sum_{i=1}^{n} \omega_i \left(\tilde{a}^\dagger(\eta_i)\tilde{a}(\eta_i) + \tilde{a}(\bar{\eta}_i)\tilde{a}^\dagger(\bar{\eta}_i)\right) = \sum_{i=1}^{n} \omega_i \tilde{a}^\dagger(\eta_i)\tilde{a}(\eta_i) + \frac{1}{2}\sum_{i=1}^{n} \omega_i.$$

The spectral analysis of H is now straightforwardly worked out, and described in any textbook on quantum mechanics. Let me recall the essentials.

It is first of all readily checked that there exists a unit vector $|0, \Omega\rangle$ in $L^2(\mathbb{R}^n)$ (unique up to a global phase), for which

$$\tilde{a}(\xi)|0, \Omega\rangle = 0, \forall \xi \in \mathbb{C}^n.$$

This common eigenvector of all the annihilation operators $\tilde{a}(\xi)$ is called the "vacuum". Remark that, as a vector in $L^2(\mathbb{R}^n)$, the vacuum $|0, \Omega\rangle$ obviously depends on Ω. One has indeed very explicitly

$$\langle x|0,\Omega\rangle = \frac{(\det\Omega)^{1/4}}{\pi^{n/4}} \exp -\frac{1}{2} x\cdot\Omega x. \tag{29}$$

Clearly $H|0,\Omega\rangle = \frac{1}{2}\sum_{i=1}^{n}\omega_i|0,\Omega\rangle$, so that the vacuum $|0,\Omega\rangle$ is actually the ground state of H. Writing for brevity $\tilde{a}_i = \tilde{a}(\eta_i), \tilde{a}_i^\dagger = \tilde{a}^\dagger(\eta_i)$ it follows (after some work) that the vectors

$$\frac{1}{\sqrt{m_1!m_2!m_3!\dots m_n!}} \left(\tilde{a}_1^\dagger\right)^{m_1} \left(\tilde{a}_2^\dagger\right)^{m_2} \left(\tilde{a}_3^\dagger\right)^{m_3} \dots \left(\tilde{a}_n^\dagger\right)^{m_n} |0,\Omega\rangle, \tag{30}$$

for all possible choices $(m_1,\dots,m_n)\in\mathbb{N}^n$ form an orthonormal basis of eigenvectors for H.

Note that the position and momentum distributions of the ground state evidently depend on Ω and are in fact not totally trivial to compute, despite the apparent simplicity of the Gaussian expression above. Indeed, if you want to know, for example, $\langle 0,\Omega|Q_7^2|0,\Omega\rangle$ you actually need to be able to diagonalize Ω^2 explicitly, and you need in particular an explicit description of the normal modes. This can be done in simple cases, such as the oscillator ring, but not in general.

One can also introduce the "number operator"

$$\tilde{N} = \sum_{i=1}^{n} \tilde{a}_i^\dagger \tilde{a}_i,$$

which commutes with H. The spectrum of $\tilde{N}$ is easily seen to equal to $\mathbb{N}$. Writing $\mathcal{E}_m$ for the eigenspace of $\tilde{N}$ with eigenvalue m, one has evidently

$$L^2(\mathbb{R}^n) = \sum_{m\in\mathbb{N}}^{\oplus} \mathcal{E}_m. \tag{31}$$

Each vector in (30) is readily checked to be an eigenvector of $\tilde{N}$ with eigenvalue $\sum_{k=1}^{n} m_k$. The preceding considerations will be the starting point for an equivalent reformulation of the quantum theory of finite dimensional oscillator systems in a manner suitable for generalization to infinite dimensional systems. This reformulation is based in an essential manner on the notion of Fock space, which I therefore first briefly recall in the next section.

3.2 Fock spaces

The basic theory of symmetric and anti-symmetric Fock spaces can be found in many places ([RS2] [BR1] are two examples) and I will not detail it here, giving only the bare essentials, mostly for notational purposes. More information on this subject can also be found in the contribution of Jan Derezinski in this volume [D].

Let $\mathcal{V}$ be a complex Hilbert space, then the Fock space $\mathcal{F}(\mathcal{V})$ over $\mathcal{V}$ is

$$\mathcal{F}(\mathcal{V}) = \overline{\oplus_{m\in\mathbb{N}}\mathcal{F}_m(\mathcal{V})},$$

where $\mathcal{F}_m(\mathcal{V})$ is the m-fold tensor product of $\mathcal{V}$ with itself. Moreover $\mathcal{F}_0(\mathcal{V}) = \mathbb{C}$. An element $\psi \in \mathcal{F}(\mathcal{V})$ can be thought of as a sequence

$$\psi = (\psi_0, \psi_1, \ldots, \psi_m, \ldots),$$

where $\psi_m \in \mathcal{F}_m(\mathcal{V})$. I will also use the notation $\mathcal{F}^{\rm fin}(\mathcal{V}) = \oplus_{m\in\mathbb{N}}\mathcal{F}_m(\mathcal{V})$, which is the dense subspace of $\mathcal{F}(\mathcal{V})$ made up of elements of the type

$$\psi = (\psi_0, \psi_1, \ldots, \psi_N, 0, 0, \ldots)$$

for some integer $N \geq 0$. Elements of $\mathcal{F}^{\rm fin}(\mathcal{V})$ will be referred to as states *with a finite number of quanta*, a terminology that I will explain later.

I will freely use the Dirac notation for Hilbert space calculations. So I will write $|\psi\rangle \in \mathcal{F}(\mathcal{V})$ as well as $\psi \in \mathcal{F}(\mathcal{V})$, depending on which one seems more convenient at any given time. Also, when no confusion can arise, I will write $\mathcal{F}_m = \mathcal{F}_m(\mathcal{V})$.

Let $\mathcal{P}_m$ be the permutation group of m elements, then for each $\sigma \in \mathcal{P}_m$, we define the unitary operator $\hat{\sigma}$ on $\mathcal{F}_m(\mathcal{V})$ by

$$\hat{\sigma}\xi_1 \otimes \xi_2 \otimes \ldots \otimes \xi_m = \xi_{\sigma^{-1}(1)} \otimes \xi_{\sigma^{-1}(2)} \otimes \ldots \otimes \xi_{\sigma^{-1}(m)},$$

($\xi_j \in \mathbb{C}^n, j = 1, \ldots, m$) and the projectors

$$P_{+,m} = \frac{1}{m!}\sum_{\sigma\in\mathcal{P}_m}\hat{\sigma}, \qquad P_{-,m} = \frac{1}{m!}\sum_{\sigma\in\mathcal{P}_m}\mathrm{sgn}(\sigma)\hat{\sigma}.$$

Now we can define the (anti-)symmetric tensor product as

$$\mathcal{F}^{\pm}_m(\mathcal{V}) = P_{\pm,m}\mathcal{F}_m(\mathcal{V})$$

whereas the (anti-)symmetric Fock space $\mathcal{F}^{\pm}(\mathcal{V})$ over $\mathcal{V}$ is

$$\mathcal{F}^{\pm}(\mathcal{V}) = \overline{\oplus_{m\in\mathbb{N}}\mathcal{F}^{\pm}_m(\mathcal{V})}.$$

Introducing the projector $P_{\pm} = \sum_{m\in\mathbb{N}} P_{\pm,m}$, we also have

$$\mathcal{F}^{\pm}(\mathcal{V}) = P_{\pm}\mathcal{F}(\mathcal{V}) \quad \text{and} \quad \mathcal{F}^{\mathrm{fin},\pm}(\mathcal{V}) = P_{\pm}\mathcal{F}^{fin}(\mathcal{V}).$$

One refers to $\mathcal{F}^{+}(\mathcal{V})$ as the symmetric or bosonic Fock space and to $\mathcal{F}^{-}(\mathcal{V})$ as the anti-symmetric or fermionic Fock space. I will only deal with the former here.

Computations in Fock space are greatly simplified through the use of "creation" and "annihilation" operators, which are abstract versions of the operators $\tilde{a}(\xi)$ and $\tilde{a}^{\dagger}(\xi)$ introduced in Sect. 3.1.

Define, for any $\xi \in \mathcal{V}$,

$$d(\xi)\xi_1 \otimes \xi_2 \ldots \otimes \xi_m = (\overline{\xi} \cdot \xi_1)\ \xi_2 \otimes \ldots \otimes \xi_m.$$

This extends by linearity and yields a well-defined bounded operator from $\mathcal{F}_m$ to $\mathcal{F}_{m-1}$ which extends to a bounded operator on all of $\mathcal{F}(\mathcal{V})$, denoted by the same symbol.

Note that I use the notation $\overline{\xi} \cdot \eta$ for the inner product on the abstract space $\mathcal{V}$ because in the applications in these notes $\mathcal{V}$ will be $\mathcal{K}^{\mathbb{C}}$, in which case this notation is particularly transparent. Of course, on a general abstract $\mathcal{V}$, there is no natural definition of "the complex conjugate $\overline{\xi}$", but that does not mean we can't use $\overline{\xi} \cdot \eta$ as a notation for the inner product.

One has $\| d(\xi) \| = \| \xi \|$. Similarly, define

$$c(\xi)\xi_1 \otimes \xi_2 \ldots \otimes \xi_m = \xi \otimes \xi_1 \otimes \xi_2 \otimes \ldots \otimes \xi_m.$$

This again yields a well-defined bounded operator from $\mathcal{F}_m$ to $\mathcal{F}_{m+1}$ which extends to a bounded operator on all of $\mathcal{F}(\mathcal{V})$, denoted by the same symbol. One has $\| c(\xi) \| = \| \xi \|$ and $d(\xi)^* = c(\xi)$.

Introducing the self-adjoint "number operator" N by

$$N\psi = (0, \psi_1, 2\psi_2, \ldots m\psi_m \ldots),$$

we can then define, on $\mathcal{F}^{\mathrm{fin}}$,

$$a_{\pm}(\xi) = P_{\pm}\sqrt{N+1}d(\xi)P_{\pm}, \qquad \text{and} \qquad a_{\pm}^{\dagger}(\xi) = P_{\pm}\sqrt{N}c(\xi)P_{\pm}.$$

The $a_{\pm}(\xi)$ are called "annihilation operators" and the $a_{\pm}^{\dagger}(\xi)$ creation operators. I will think of $a_{-}(\xi)$ as an operator on $\mathcal{F}^{-}$ and of $a_{+}(\xi)$ as an operator on $\mathcal{F}^{+}$. Direct computation (on $\mathcal{F}^{fin}$, for example) yields the following crucial commutation and anti-commutation relations between those operators:

$$[a_+(\xi_1), a_+(\xi_2)] = 0 = [a_+^{\dagger}(\xi_1), a_+^{\dagger}(\xi_2)], \qquad [a_+(\xi_1), a_+^{\dagger}(\xi_2)] = \overline{\xi_1} \cdot \xi_2, \quad (32)$$

Those are referred to as the canonical commutation relations or CCR. You should compare (32) to (26) and be amazed.

Working in the bosonic Fock space $\mathcal{F}^{+}$ and using the above relations one establishes through direct computation that

$$\sqrt{m!}P_+\xi_1 \otimes \xi_2 \otimes \ldots \otimes \xi_m = a_+^{\dagger}(\xi_1)a_+^{\dagger}(\xi_2)\ldots a_+^{\dagger}(\xi_m)|0\rangle.$$

Here I introduced the notation $|0\rangle = (1, 0, 0, \ldots) \in \mathcal{F}_0 \subset \mathcal{F}$. This vector is usually referred to as the Fock vacuum or simply as the vacuum. It can be characterized as being the unique vector in $\mathcal{F}^{+}$ for which

$$a_+(\xi)|\psi\rangle = 0, \qquad \forall \xi \in \mathcal{V}.$$

For explicit computations and in order to understand the physics literature, it is a Good Thing to have a convenient basis at hand. So suppose you have an orthonormal basis η_j of $\mathcal{V}$ (with $j = 1, 2, \ldots \dim\mathcal{V}$). Then you can define, for

any positive integer $k \leq \dim\mathcal{V}$ and for any choice of $(m_1, m_2, m_3, \ldots, m_k) \in \mathbb{N}^k$, the vector

$$|m_1, m_2, m_3, \ldots, m_k\rangle := (m_1!m_2!\ldots m_k!)^{-1/2} \times \left(a_+^\dagger(\eta_1)\right)^{m_1} \left(a_+^\dagger(\eta_2)\right)^{m_2} \left(a_+^\dagger(\eta_3)\right)^{m_3} \ldots \left(a_+^\dagger(\eta_k)\right)^{m_k} |0\rangle. \tag{33}$$

Those vectors are now easily checked to form an orthonormal basis of $\mathcal{F}^+$. The numbers m_j are often referred to as the "occupation numbers" of the states η_j. Note that each of them is an eigenvector of the number operator with eigenvalue given by $\sum_{j=1}^k m_j$.

It is a good exercise to prove that $N_+ = P_+ N P_+$, the restriction of the number operator to $\mathcal{F}^+$ can be written

$$N_+ = \sum_j a_+^\dagger(\eta_j) a_+(\eta_j).$$

If U is a unitary operator on $\mathcal{V}$, the unitary operator $\Gamma(U)$ on $\mathcal{F}^+$ is defined as $\otimes_{k=1}^m U$ when restricted to $\mathcal{F}_m^+$. When A is a self-adjoint operator on $\mathcal{V}$, $\mathrm{d}\Gamma(A)$ is the self-adjoint operator on $\mathcal{F}^+$ defined as

$$A \otimes \mathbb{1} \otimes \ldots \otimes \mathbb{1} + \mathbb{1} \otimes A \otimes \ldots \otimes \mathbb{1} + \ldots + \mathbb{1} \otimes \ldots \otimes \mathbb{1} \otimes A$$

on (a suitable domain) in $\mathcal{F}_m^+$, for each $m > 0$. Also $\mathrm{d}\Gamma(A)\mathcal{F}_0^+ = 0$. It is a good exercise to check that, if A has a basis of eigenvectors

$$A\eta_j = \alpha_j \eta_j$$

then

$$\mathrm{d}\Gamma(A) = \sum_i \alpha_i \; a_+^\dagger(\eta_i) a_+(\eta_i).$$

3.3 The Fock representation: finite dimensional fields

It is now straightforward to reformulate the quantum description of the oscillator system in Sect. 3.1 as follows. First of all, in view of (31) and the considerations of the previous section, it is clear that there exists a unitary map T_Ω

$$T_\Omega : L^2(\mathbb{R}^n) \to \mathcal{F}^+(\mathbb{C}^n)$$

satisfying

$$T_\Omega \mathcal{E}_m = \mathcal{F}_m^+(\mathbb{C}^n), \quad T_\Omega H T_\Omega^{-1} = \mathrm{d}\Gamma(\Omega) + \frac{1}{2}\sum_{i=1}^n \omega_i,$$

and

$$T_\Omega \tilde{a}(\xi) T_\Omega^{-1} = a_+(\xi),$$

for all $\xi \in \mathbb{C}^n$. In fact, quite explicitly, one has, for all $\xi_1, \xi_2, \ldots \xi_m \in \mathbb{C}^n$,

$$T_\Omega : \tilde{a}^\dagger(\xi_1) \ldots \tilde{a}^\dagger(\xi_m)|0, \Omega\rangle \in \mathcal{E}_m \subset L^2(\mathbb{R}^n) \\ \mapsto a_+^\dagger(\xi_1) \ldots a_+^\dagger(\xi_m)|0\rangle \in \mathcal{F}_m^+(\mathbb{C}^n) \subset \mathcal{F}^+(\mathbb{C}^n).$$

The unitary map T_Ω transports each object of the theory from $L^2(\mathbb{R}^n)$ to the symmetric Fock space over $\mathbb{C}^n$ and provides in this manner an equivalent quantum mechanical description of the oscillator system, that goes under the name of Fock representation.

Note that in the left hand side of the above equations, the operators $\tilde{a}(\xi)$ or $\tilde{a}^\dagger(\xi)$ are the concrete differential operators on $L^2(\mathbb{R}^n)$ that were defined in (25) and that depend explicitly on Ω. In the right hand side, you find the abstract creation and annihilation operators defined in Sect. 3.2. Note that those do not depend on Ω at all. Similarly, the ground state vector $|0, \Omega\rangle$ of H appearing in the left hand side is of course Ω-dependent, whereas the Fock vacuum $|0\rangle$ in the right hand side is not. This is somewhat paradoxical. Indeed, since the vacuum is the ground state of the Hamiltonian, should it not depend on this Hamiltonian? The answer to this conundrum goes as follows, and is very similar to the discussion in Sect. 2.4 in the classical context. Recall that it is customary to say that each physical state of the system is represented by a vector in a Hilbert space. Consider for example the vacuum vector $|0\rangle$ in Fock space. To find out to which physical state of the system it corresponds, one has to compute the expectation value of physical observables in this state. Now, for a system of coupled oscillators, the most relevant observables are arguably the coordinates of position and momentum. In view of (27) and (28) it is now clear that

$$T_\Omega \eta \cdot Q T_\Omega^{-1} = \frac{1}{\sqrt{2}}(a_+(\Omega^{-1/2}\overline{\eta}) + a_+^\dagger(\Omega^{-1/2}\eta)), \tag{34}$$

and, similarly,

$$T_\Omega \eta \cdot P T_\Omega^{-1} = \frac{i}{\sqrt{2}}(a_+^\dagger(\Omega^{1/2}\eta) - a_+(\Omega^{1/2}\overline{\eta})). \tag{35}$$

I will in the following not hesitate to write $T_\Omega \eta \cdot Q T_\Omega^{-1} = \eta \cdot Q$ and $T_\Omega \eta \cdot P T_\Omega^{-1} = \eta \cdot P$, in agreement with the usual convention that consists of not making the identification operator T_Ω notationally explicit. But it is now clear that, contrary to what happens on $L^2(\mathbb{R}^n)$, the explicit expression of the position and momentum observables as operators on Fock space depends on the dynamics, via Ω! Hence the expectation values of those operators, and of polynomial expressions in these operators will also depend on Ω. In this sense, *the same mathematical object*, namely the vector $|0\rangle \in \mathcal{F}^+(\mathbb{C}^n)$ *corresponds to a different physical state of the system* of n coupled oscillators for different choices of Ω, *i.e.* of the spring constants. Also, the *same physical*

quantity, such as the displacement of the seventh oscillator, is represented by a different mathematical operator, namely the operator in the right hand side of (34), with $\eta(j) = \delta_{j7}$. In particular, if you are interested in the mean square displacement of the seventh oscillator when the system is in the ground state, *i.e.* $\langle 0|Q_7^2|0\rangle$, you will need a detailed spectral analysis of Ω and in particular a good understanding of the spatial distribution of its normal modes over the n degrees of freedom of the system, as I already pointed out. The result you find will of course depend on Ω.

In the same manner, any other given fixed vector in the Fock space, such as for example a state of the form $a_+^\dagger(\xi)|0\rangle$, for some fixed choice of $\xi \in \mathbb{C}^n$, represents a *different* physical state depending on Ω.

In short, the interpretation of a given vector in Fock space as a state of a physical system depends on the dynamics of the system under consideration because the representation of the physical observables of the system by operators on Fock space is dynamics dependent.

To avoid confusion, these simple remarks need to be remembered when dealing with the infinite dimensional theory, where only the Fock representation survives. In particular, the name "vacuum vector" or "vacuum state" given to the Fock vacuum conveys the wrong idea that, somehow, when the system state is represented by this vector, space is empty, there is "nothing there" and therefore this state should have trivial physical properties that in fact should be independent of the system under consideration and in particular of the dynamics.

3.4 The Fock representation: general free fields

Summing up, we have now reformulated the quantum mechanical description of a finite dimensional coupled oscillator system in a way that will be seen to carry over immediately – with only one moderate change – to the infinite dimensional case. Indeed, given a free oscillator field determined by $\mathcal{K}$ and Ω, it is now perfectly natural to choose as the quantum Hilbert space of such a system the Fock space $\mathcal{F}^+(\mathcal{K}^{\mathbb{C}})$, and as quantum Hamiltonian $H = \mathrm{d}\Gamma(\Omega)$. Note that this is a positive operator and that the Fock vacuum is its ground state, with eigenvalue 0. Proceeding in complete analogy with the finite dimensional case, the quantization of the classical creation and annhilition functions $a_{\mathrm{c}}(\xi), a_{\mathrm{c}}^\dagger(\xi)$ are the creation and annihilation operators $a_+(\xi), a_+^\dagger(\xi)$. In terms of those the quantized fields and their conjugates are then *defined* precisely as before ($\eta \in \mathcal{K}^{\mathbb{C}}_{-1/2}$):

$$\eta \cdot Q := \frac{1}{\sqrt{2}}(a_+(\Omega^{-1/2}\eta) + a_+^\dagger(\Omega^{-1/2}\eta)), \tag{36}$$

and, similarly ($\eta \in \mathcal{K}^{\mathbb{C}}_{1/2}$),

$$\eta \cdot P := \frac{\mathrm{i}}{\sqrt{2}}(a_+^\dagger(\Omega^{1/2}\eta) - a_+(\Omega^{1/2}\overline{\eta})). \tag{37}$$

It is often convenient to think of "the field Q" as the map that associates to each $\eta \in \mathcal{K}_{-1/2}$ the self-adjoint operator in the right hand side of (36), and similarly for "the conjugate field P", defined on $\mathcal{K}_{1/2}$. With this language, the field operator $\eta \cdot Q$ is the value of the field Q at $\eta \in \mathcal{K}_{-1/2}$. This notation is reasonable since the field is a linear function of its argument.

The moderate change to which I referred to above is the fact that, if I compare the above quantization prescription for the case $\mathcal{K} = \mathbb{R}^n$ to the one of Sect. 3.1 and Sect. 3.3, then it is clear that I substracted from the Hamiltonian the "zero-point energy", $\sum_{i=1}^n \omega_i$. It is argued in all quantum field theory texts that this constitutes an innocuous change, for two distinct reasons. First, adding a constant to the Hamiltonian does not change the dynamics in any fundamental way. Second only energy differences count in physics, so tossing out an additive constant in the definition of the energy should not change anything fundamentally. As a result, since the expression $\sum_{i=1}^n \omega_i$ makes no sense in general in infinite dimensions, where it is formally typically equal to $+\infty$, it seems like a good idea to toss it out from the very beginning! This means you calibrate the energy so that the ground state of the system, which is represented by the Fock vacuum, has zero *total* energy, independently of Ω, and leads to the choice of $H = \mathrm{d}\Gamma(\Omega)$ as the Hamiltonian.

While this is the reasoning found in all physics and mathematical physics texts the tossing out of the zero-point energy is not such an innocent operation after all. For the physics of the zero-point energy, I refer to [Mi]. See also [DB2] for further comments.

It is instructive to compute the evolution of the field and the conjugate field under the dynamics. Since

$$\mathrm{e}^{-\mathrm{i}Ht} = \Gamma(\mathrm{e}^{-\mathrm{i}\Omega t}),$$

it is easy to check that

$$\mathrm{e}^{\mathrm{i}Ht} a_+(\xi) \mathrm{e}^{-\mathrm{i}Ht} = a_+(\mathrm{e}^{\mathrm{i}\Omega t}\xi).$$

Define then the evolved field $Q(t)$ as the map that associates to each $\eta \in \mathcal{K}_{-1/2}$ the self-adjoint operator $\eta \cdot Q(t)$ defined as follows:

$$\eta \cdot Q(t) \equiv \mathrm{e}^{\mathrm{i}Ht}(\eta \cdot Q)\mathrm{e}^{-\mathrm{i}Ht}.$$

A simple computation then yields

$$\eta \cdot Q(t) = \frac{1}{\sqrt{2}}(a_+(\Omega^{-1/2}\mathrm{e}^{\mathrm{i}\Omega t}\overline{\eta}) + a_+^\dagger(\Omega^{-1/2}\mathrm{e}^{\mathrm{i}\Omega t}\eta)).$$

Hence

$$\frac{\mathrm{d}^2}{\mathrm{d}t^2}\eta \cdot Q(t) = -\Omega^2 \eta \cdot Q(t).$$

One defines similarly $\eta \cdot P(t)$, which obeys the same equation. In fact, $\eta \cdot Q(t)$ and $\eta \cdot P(t)$ are operator-valued solutions of this with $\eta \cdot Q(t)$ satisfying the

equal time commutation relations. They are called the Heisenberg field and conjugate field in the physics literature.

We are now in a position to further study these systems, a task I turn to next. First, a word on the "particle interpretation of the field states" is in order.

3.5 Particle interpretation of the field states

Physicists refer to $\mathcal{F}_m$ as the m particle sector of the Fock space ($m \geq 1$) and to $\mathcal{F}_0$ as the vacuum sector. This terminology comes from the following remark. As any beginners' text in quantum mechanics will tell you, whenever the quantum Hilbert space of a single particle (or a single system) is $\mathcal{V}$, the Hilbert space of states for m (identical) particles (or systems) is the m-fold tensor product of $\mathcal{V}$. The simplest case is the one where $\mathcal{V} = L^2(\mathbb{R}^d)$. Then the m-fold tensor product can be naturally identified with $L^2(\mathbb{R}^d \times \ldots \times \mathbb{R}^d = \mathbb{R}^{dm})$, which is isomorphic to $\otimes_m \mathcal{V}$. The same quantum mechanics course will teach you that, when the particles are indistinguishable, the state space needs to be restricted either to the symmetric or anti-symmetric tensor product. In the first case, which is the one we are dealing with here, the particles are said to be bosons, otherwise they are fermions. In the case where $\mathcal{V} = L^2(\mathbb{R}^d)$, the m-fold symmetric tensor product of $\mathcal{V}$ consists of all symmetric L^2-functions of m variables.

The above considerations suggest that, *conversely*, whenever the quantum state space of a physical system turns out to be a Fock space over some Hilbert space $\mathcal{V}$, one may think of $\mathcal{V}$ as a one-particle space, and of $\mathcal{F}_m(\mathcal{V})$ as the corresponding m-particle space. An arbitrary state of the system can then be thought of as a superposition of states with 0, 1, 2, ... m, ... particles. These ideas emerged very quickly after the birth of quantum mechanics, as soon as physicists attacked the problem of analyzing the quantum mechanical behaviour of systems with an infinite number of degrees of freedom, such as the electromagnetic field. The Fock space structure of the Hilbert space of states describing the *field* immediately lead to such an interpretation in terms of *particles*. For the electromagnetic field, the particles were baptized "photons", and in complete analogy, the quantum mechanical description of lattice vibrations in solid state physics lead to the notion of "phonons". The idea that one can associate a particle interpretation to the states of a Fock space is further corroborated by the observation that those states carry energy and momentum in "lumps". This can be seen as follows. Suppose, in our notations, that Ω has a pure point spectrum:

$$\Omega\eta_j = \omega_j\eta_j,\ j \in \mathbb{N}.$$

Then the quantum Hamiltonian is

$$H = \mathrm{d}\Gamma(\Omega) = \sum_j \omega_j a_j^\dagger a_j,$$

where I wrote $a_j^\dagger = a^\dagger(\eta_j)$. Note that I have dropped the index + on the creation and annihilation operators, a practice that I shall stick to in what follows since I will at any rate be working on the symmetric Fock space all the time. Now consider for example the state

$$a_1^\dagger (a_5^\dagger)^3 a_{10}^\dagger |0\rangle.$$

This is a 5-particle state, and an eigenvector of the Hamiltonian with eigenvalue $\omega_1 + 3\omega_5 + \omega_{10}$. It is natural to think of it intuitively as being a state "containing" 3 particles of energy ω_5, and one particle of energy ω_1 and ω_{10} each. Similarly, in translationally invariant systems, such states can be seen to carry a total momentum which is the sum of "lumps" of momentum corresponding to its individual constituents. Of course, the particle interpretation of the states of the field is a very important feature of the theory since it is essential for the interpretation of high energy experiments, and so it has quite naturally received a lot of attention.

Despite its undeniable value, the suggestive interpretation of the states of Fock space in terms of particles may lead (and has lead) to some amount of confusion and has to be taken with a (large) grain of salt. Some of those problems seem to have been brought out clearly only when physicists started to investigate quantum field theory on curved space-times. A critical discussion of this issue can be found throughout [Fu]. Although Fulling does adopt the second quantization viewpoint, he stresses repeatedly the need to escape "from the tyranny of the particle concept" in order to "come to a completely field theoretic understanding of quantum field theory." Similarly, Wald, who does indeed adopt a field theoretic viewpoint throughout in [Wa], gives a critical analysis of the merits and limitations of the particle concept in quantum field theory. He actually stresses the need to "unlearn" some of the familiar concepts of quantum field theory on flat space times to understand the curved space time version of the theory.

There are in fact several sources of problems with the particle interpretation of the states in quantum field theory. The first one was already hinted at in Sect. 3.3: the use of the word "vacuum" to describe the ground state of the system invites one to think that when the system is in this state, there is "nothing there". Actually, one may be tempted to think the system itself is simply not there! But to see that makes no sense, it is enough to think of an oscillator lattice. Certainly, when this system is in its ground state, all oscillators are there! It is just that the system is not excited, so there are no "particles" in the above (Fock space) sense of the word, and this in spite of the fact that the mechanical particles making up the lattice are certainly present. Also, if one thinks of the vacuum state as empty space, it becomes impossible to understand how its properties can depend on the system considered via Ω. In fact, it is quite baffling to think "empty space" could have any properties at all. In particular, the mean square displacement of the field, for example, given by

$$\langle 0|(\eta \cdot Q)^2|0\rangle$$

is a function of Ω, as is easily seen even in finite dimensional oscillator systems. This quantity is an example of a so-called "vacuum fluctuation". Of course, for systems with a finite number of degrees of freedom, we find this phenomenon perfectly natural, but if you study the Klein-Gordon field, for example, and call the ground state the vacuum, you end up being surprised to see vacuum expectation values depend on the mass of particles that are not there!

A second source of confusion is that the notion of "particle" evokes a localized entity, carrying not only momentum and energy, but that one should also be able to localize in space, preferably with the help of a position operator. I will show in Section 4 that there is no reasonable notion of "position" that can be associated to the one-particle states of Fock space, contrary to what happens in the usual non-relativistic quantum mechanics of systems with a finite number of particles. In particular, there is no reasonable "position operator". This has nothing to do with relativity, but is true for large classes of Ω and in particular for all examples given so far. So even if the particles of field theory share a certain number of properties with the usual point particles of classical and quantum mechanical textbooks, they have some important features that make them quite different. They are analogous objects, but not totally similar ones. This, I will argue, has nothing to do either with special or general relativity, but is clear if one remembers systematically the analogy with finite dimensional oscillator systems.

As a constant reminder of the fact that the so-called particles of quantum field theory are nothing but excitations of its ground state, it is a good idea to use the older physics terminology and to talk systematically of "quasi-particles", "quanta", "field quanta" or of "elementary excitations of the field" rather than simply of particles when describing the states of Fock space. I will adhere as much as possible to this prudent practice.

Moreover, when testing your understanding of a notion in quantum field theory, try to see what it gives for a finite system of oscillators. If it looks funny there, it is likely to be a bad idea to use it in the infinite dimensional case.

The remaining parts of this section develop material that will be needed in Section 4. It is perhaps a good idea to start reading the latter, coming back to this material only as I refer to it.

3.6 Weyl operators and coherent states

Given a Hilbert space $\mathcal{V}$ and the corresponding symmetric Fock space $\mathcal{F}^+(\mathcal{V})$, we can first define, for any $\xi \in \mathcal{V}$, the *Weyl operator*

$$W_{\mathrm{F}}(\xi) = \mathrm{e}^{a^\dagger(\xi) - a(\xi)}.$$

A coherent state is then defined as a vector of $\mathcal{F}^+(\mathcal{V})$ of the form

$$|\xi\rangle \stackrel{\mathrm{def}}{=} W_{\mathrm{F}}(\xi)|0\rangle,$$

for some $\xi \in \mathcal{V}$. Note that the map

$$\xi \in \mathcal{V} \mapsto |\xi\rangle \in \mathcal{F}^+(\mathcal{V})$$

provides a *nonlinear* imbedding of $\mathcal{V}$ into $\mathcal{F}^+(\mathcal{V})$ which is not to be confused with the trivial linear imbedding $\mathcal{V} \cong \mathcal{F}_1(\mathcal{V}) \subset \mathcal{F}^+(\mathcal{V})$. Given an arbitrary $0 \neq \psi \in \mathcal{V}$, one can likewise consider the family $W_{\rm F}(\xi)\psi$, and those vectors are also referred to as a family of coherent states.

Coherent states play an important role in the semi-classical analysis of quantum systems and in various branches of theoretical physics [KSk] [Pe]. We describe them here in the abstract context of symmetric Fock spaces. They are very simple objects to define but nevertheless have an seemingly inexhaustable set of interesting properties. I will only mention those I need.

To compute with the coherent states, we need a number of formulas that are listed below and that can all be obtained easily, if one remembers first of all that, if A and B are bounded operators so that $C = [A, B]$ commutes with both A and B, then

$$\mathrm{e}^{A+B} = \mathrm{e}^{A}\mathrm{e}^{B}\mathrm{e}^{-\frac{C}{2}}, C = [A, B].$$

Computing with $a^\dagger(\xi)$ and $a(\xi)$ as if they were bounded operators, all formulas below follow from this and some perseverance in computing. Taking care of the domain problems to make them completely rigorous is tedious but character building and can be done using the techniques described in [BR2] or [RS2]. First of all, we have, for all $\xi_1, \xi_2 \in \mathcal{V}$,

$$W_{\rm F}(\xi_1)W_{\rm F}(\xi_2) = W_{\rm F}(\xi_1 + \xi_2)\mathrm{e}^{-\mathrm{i}\mathrm{Im}(\overline{\xi}_1 \cdot \xi_2)}.$$

As a result

$$W_{\rm F}(\xi_1)W_{\rm F}(\xi_2) = W_{\rm F}(\xi_2)W_{\rm F}(\xi_1)\mathrm{e}^{-2\mathrm{i}\mathrm{Im}(\overline{\xi}_1 \cdot \xi_2)},$$

and

$$[W_{\rm F}(\xi), W_{\rm F}(\xi')] = W_{\rm F}(\xi')W_{\rm F}(\xi)\left(\mathrm{e}^{\mathrm{i}2\mathrm{Im}(\overline{\xi}' \cdot \xi)} - 1\right).$$

Furthermore

$$W_{\rm F}(s\xi)W_{\rm F}(\xi')W_{\rm F}(t\xi) = W_{\rm F}((s+t)\xi)W_{\rm F}(\xi')\mathrm{e}^{2\mathrm{i}t\mathrm{Im}(\overline{\xi} \cdot \xi')}$$

and hence

$$W_{\rm F}(-\zeta)W_{\rm F}(\xi)W_{\rm F}(\zeta) = W_{\rm F}(\xi)\mathrm{e}^{\mathrm{i}2\mathrm{Im}(\overline{\zeta} \cdot \xi)},$$

or

$$W_{\rm F}(-\zeta)W_{\rm F}(\xi)W_{\rm F}(\zeta) = \mathrm{e}^{\left[(a^\dagger(\xi) + \xi \cdot \overline{\zeta}) - (a(\xi) + \overline{\xi} \cdot \zeta)\right]}.$$

One then finds

$$W_{\rm F}(-\zeta)\left[a^\dagger(\xi)\right]^n W_{\rm F}(\zeta) = (a^\dagger(\xi) + \xi \cdot \overline{\zeta})^n,\ W_{\rm F}(-\zeta)a^n(\xi)W_{\rm F}(\zeta) = (a(\xi) + \overline{\xi} \cdot \zeta)^n.$$

It is often convenient to write

$$W_{\rm F}(\xi) = {\rm e}^{a^\dagger(\xi)}{\rm e}^{-a(\xi)}{\rm e}^{-\frac{1}{2}\|\xi\|^2} = {\rm e}^{-a(\xi)}{\rm e}^{a^\dagger(\xi)}{\rm e}^{\frac{1}{2}\|\xi\|^2}.$$

Also, remark that, for all $\xi \neq 0$,

$$\| W_{\rm F}(\xi) - \mathbb{1} \| = 2 \text{ and } {\rm s} - \lim_{t\to 0} W_{\rm F}(t\xi) = \mathbb{1}.$$

Using what precedes, one easily finds the following formulas involving the vacuum.

$$|\xi\rangle = {\rm e}^{-\frac{1}{2}\|\xi\|^2}{\rm e}^{a^\dagger(\xi)}|0\rangle, \tag{38}$$

$$\langle 0|a^n(\xi)|\xi'\rangle = {\rm e}^{-\frac{1}{2}\|\xi'\|^2}(\overline{\xi}\cdot\xi')^n, \tag{39}$$

and

$$\langle\zeta|W_{\rm F}(\xi)|\zeta\rangle = {\rm e}^{-\frac{1}{2}\|\xi\|^2}{\rm e}^{{\rm i}2{\rm Im}(\overline{\zeta}\cdot\xi)}. \tag{40}$$

3.7 Observables and observable algebras

Physically measurable quantities of a system are, in its classical description, represented by functions on phase space. Consider first finite dimensional systems. An example, in the case of an oscillator ring, is "the displacement of the ninth oscillator", represented by $q_9 : X = (q,p) \in \mathcal{H} \to q_9 \in \mathbb{R}$. Some interesting observables are represented by linear functions (such as position and momentum) or by quadratic functions (such as energy or angular momentum). More generally, they may be polynomial. To discuss the linear functions, it is helpful to notice that the *topological* dual space of $\mathcal{H}$ can conveniently be identified with $\mathcal{H}$ itself using the symplectic form: to each $Y \in \mathcal{H}$, we associate the linear map

$$X \in \mathcal{H} \mapsto s(Y,X) \in \mathbb{R}.$$

One has, from (8), for every $Y_1, Y_2 \in \mathcal{H}$,

$$\{s(Y_1,\cdot),\ s(Y_2,\cdot)\} = s(Y_1,Y_2). \tag{41}$$

It is then convenient to introduce

$$V_{\rm c}(Y) = {\rm e}^{-{\rm i}s(Y,\cdot)} \tag{42}$$

which serves as a generating function for monomials of the type

$$s(Y_1,\cdot)s(Y_2,\cdot)\dots s(Y_n,\cdot) = \frac{(i\partial)^n}{\partial t_1\partial t_2\dots\partial t_n} V_{\rm c}(t_1Y_1 + \dots t_nY_n)_{|t_1=0=t_2\dots=t_n}.$$

It is immediate from the definition of the $V_c(Y)$ that

$$V_{\rm c}(Y)\circ\Phi_t = V_{\rm c}(\Phi_{-t}Y).$$

Working in the Schrödinger representation, the quantum mechanical analogues of the $V_{\rm c}(Y)$ are the Weyl operators

$$V(Y) = \mathrm{e}^{-\mathrm{i}(a\cdot P - b\cdot Q)}, \text{ where } Y = (a,b) \in \mathcal{H}. \tag{43}$$

The $V(Y)$ are clearly unitary operators on $L^2(\mathbb{R}^n)$ and satisfy the so-called Weyl relations

$$V(Y_1)V(Y_2) = \mathrm{e}^{-\frac{\mathrm{i}}{2}s(Y_1,Y_2)}V(Y_1+Y_2), \qquad \forall\, Y_1, Y_2 \in \mathcal{H}.$$

In a Fock representation (determined by a choice of Ω), one has, with the notation of Sect. 3.3

$$T_\Omega V(Y) T_\Omega^{-1} = W_{\mathrm{F}}(z_\Omega(Y)).$$

Here the $W_{\mathrm{F}}(z_\Omega(Y))$ are the Weyl operators on the symmetric Fock space $\mathcal{F}^+(\mathbb{C}^n)$, as introduced in Sect. 3.6.

In the algebraic approach to quantum theory, one postulates that the interesting observables of the theory include at least those that can be written as finite sums of $V(Y)$. One therefore considers the algebra

$$\mathrm{CCR}_0(\mathbb{R}^{2n}) = \text{span}\,\{W_{\mathrm{F}}(z_\Omega(Y)) \mid Y \in \mathbb{R}^{2n}\} = \text{span}\,\{W_{\mathrm{F}}(\xi) \mid \xi \in \mathbb{C}^n\}.$$

This algebra is irreducible. This means that the only closed subspaces of $L^2(\mathbb{R}^n) \cong \mathcal{F}^+(\mathbb{C}^n)$ invariant under the above algebra are the trivial ones and is equivalent, via Schur's Lemma, to the statement that the only bounded operators that commute with all F in the algebra are the multiples of the identity. For a simple proof of these facts one may consult [DB1]. This implies via a well known result in the theory of von Neumann algebras (see [BR1], for example) that its weak closure is all of $\mathcal{B}(\mathcal{F}^+(\mathbb{C}^n))$: in this sense, "any bounded operator on Fock space can be approximated (in the weak topology!) by a function of Q and P." This is clearly a way of saying that the original algebra is quite large. Note nevertheless that its operator norm closure (called the CCR-algebra over $\mathbb{R}^{2n}$ and denoted by $\mathrm{CCR}(\mathbb{R}^{2n})$) is much smaller, since it contains no compact operators. For the purposes of these notes, I will consider $\mathrm{CCR}(\mathbb{R}^{2n})$ or $\mathrm{CCR}_0(\mathbb{R}^{2n})$ as "the" observable algebra of the systems considered.

Remark that these algebras do, as sets, not depend on Ω. But again, in close analogy to what we observed in Sect. 3.3, given an operator on Fock space belonging to one of these algebras, its expression in terms of Q and P does depend on Ω, and so does therefore its physical interpretation as an observable. So it is not only the identification of the appropriate observable algebra which is important, but the labeling, within this algebra, of the elements that describe the relevant physical observables. This will be crucial once we discuss local observables in Section 4, and become hopefully quite a bit clearer then too.

It is obviously not of much interest to discuss observable algebras if one is not going to say how the observables evolve in time. In finite dimensional systems, one is given a Hamiltonian H, which is a self-adjoint operator on

$L^2(\mathbb{R}^n) \cong \mathcal{F}^+(\mathbb{C}^n)$. It generates the so-called Heisenberg evolution of each observable F, which is defined by $\alpha_t(F) = \mathrm{e}^{\mathrm{i}\mathrm{i}Ht}F\mathrm{e}^{-\mathrm{i}Ht}$. It has to be checked that the algebra of observables and H are such that this defines an automorphism of the algebra (*i.e.* so that $\mathrm{e}^{\mathrm{i}Ht}F\mathrm{e}^{-\mathrm{i}Ht}$ still belongs to the algebra if F does).

That α_t is an automorphism of the CCR algebra is not true in general. For example, it is proven in [FV] that, when $H(\lambda) = \frac{1}{2}P^2 + \lambda V$, with V a bounded L^1 function, then the Heisenberg evolution leaves the CCR algebra invariant for all values of t and of λ if and only if $V = 0$. In other words, the CCR algebra cannot possibly be a suitable algebra to describe most standard quantum mechanical systems with a finite number of degrees of freedom.

An exception to this rule are systems described by quadratic hamiltonians, which are precisely the ones we are interested in here. An easy example is provided by quadratic Hamiltonians of the type $H = \frac{1}{2}P^2 + \frac{1}{2}Q \cdot \Omega^2 Q$ in view of

$$\mathrm{e}^{\mathrm{i}\mathrm{d}\Gamma(\Omega)t}W_{\mathrm{F}}(\xi)\mathrm{e}^{-\mathrm{i}\mathrm{d}\Gamma(\Omega)t} = W_{\mathrm{F}}(\mathrm{e}^{-\mathrm{i}\Omega t}\xi),\ \forall \xi \in \mathcal{K}^{\mathbb{C}},$$

which follows immediately from the discussion in Sect. 3.4. This clearly implies that the dynamics leaves the CCR algebra $\mathrm{CCR}(\mathbb{R}^{2n})$ invariant. Note that this will work in infinite dimensional systems just as well as in finite dimensional ones.

The discussion carries over to the infinite dimensional case without change. One defines the algebra of observables in the quantum theory to be

$$\mathrm{CCR}_0(\mathcal{H}) = \mathrm{span}\ \{W_{\mathrm{F}}(z_\Omega(Y)) \mid Y \in \mathcal{H}\} = \mathrm{span}\ \{W_{\mathrm{F}}(\xi) \mid \xi \in \mathcal{K}^{\mathbb{C}}\}.$$

Again, this algebra is independent of Ω and turns out to be irreducible [BR1], so that its weak closure is the algebra of all bounded operators on Fock space. Its norm closure, which is much smaller, is the so-called CCR-algebra over $\mathcal{H}$, for which I will write $\mathrm{CCR}(\mathcal{H})$. Since we will only work with quadratic Hamiltonians, this algebra is adequate for the description of such systems since it is then invariant under the dynamics. Here also, to no one's surprise by now, I hope, the interpretation of a given operator in the algebra as an observable *will* depend on Ω, as we will see in more detail in Section 4.

For further reference, let me define also the algebra

$$\mathrm{CCR}_0(\mathcal{M}) = \mathrm{span}\ \{W_{\mathrm{F}}(z_\Omega(Y))|Y \in \mathcal{M}\},$$

whenever $\mathcal{M}$ is a vector subspace of $\mathcal{H}$ (even if $\mathcal{M}$ is not symplectic). In many situations it is natural and elegant not to work with the norm closure of the $\mathrm{CCR}_0(\mathcal{M})$, but with their weak closure, for which I shall write $\mathrm{CCR}_{\mathrm{w}}(\mathcal{M})$. Further developments concerning the CCR can be found in the contribution of J. Dereziński in this volume [D].

4 Local observables and local states

4.1 Introduction

The issue of what are local observables, local states and local measurements has attracted a fair amount of attention and has generated some surprises and even some controversy in the mathematical physics literature on relativistic quantum field theory. The controversy has centered on the question of particle localization, of possible causality violations and of relativistic invariance. I will address these issues in the present section within the restricted context of the free oscillator fields under study here, some of which are relativistically invariant, while others are not. I will argue that there is not much reason to be surprised and certainly no ground for controversy.

After defining what is meant by a local observable (Sect. 4.2) and giving some examples (Sect. 4.3), the notion of "strictly local excitation of the vacuum" is introduced in Sect. 4.4. I will then state a generalization of a theorem of Knight asserting that, if Ω is a non-local operator, then states with a finite number of field excitations cannot be strictly local excitations of the vacuum (Sect. 4.5). It will be shown through examples (Sect. 4.6) that the above condition on Ω is typically satisfied in models of interest and I will explain the link between the above notion of localized excitation of the vacuum and the so-called Newton-Wigner localization (Sect. 4.7). It will be argued that the latter is not a suitable notion to discuss the local properties of the states of oscillator fields. The actual proof of Knight's theorem is deferred to Sect. 4.8.

4.2 Definition of a local structure

Among the interesting observables of the oscillator systems we are studying are certainly the "local" ones. I will give a precise definition in a moment, but thinking again of the oscillator chain, "the displacement q_7 of the seventh oscillator" is certainly a "local" observable. In the same way, if dealing with a wave equation, "the value $q(x)$ of the field at x " is a local observable. The Hamiltonian is on the other hand not a local observable, since it involves sums or integrals over all oscillator displacements and momenta. Generally, "local observables" are functions of the fields and conjugate fields in a bounded region of space. Of course, this notion does not make sense for all harmonic systems, defined by giving a positive operator Ω^2 on some abstract Hilbert space $\mathcal{K}$. So let me reduce the level of abstractness of the discussion, therefore hopefully increasing its level of pertinence, and define what I mean by a system with a local structure.

In view of what precedes, I will limit my attention to free oscillator fields over a real Hilbert space $\mathcal{K}$ of the form $\mathcal{K} = L^2_{\mathbb{R}}(K, \mathrm{d}\mu)$, where K is a topological space and μ a Borel measure on K. Here the subscript "$\mathbb{R}$" indicates that we are dealing with the real Hilbert space of real-valued functions. In fact, all examples I have given so far are of the above type.

Definition 1. *A local structure for the oscillator field determined by Ω and $\mathcal{K} = L^2_{\mathbb{R}}(K, \mathrm{d}\mu)$ is a subspace $\mathcal{S}$ of $\mathcal{K}$ with the following properties:*

1. $\mathcal{S} \subset \mathcal{K}_{1/2} \cap \mathcal{K}_{-1/2}$;
2. *Let B be a Borel subset of K, then $\mathcal{S}_B \equiv \mathcal{S} \cap L^2_{\mathbb{R}}(B, \mathrm{d}\mu)$ is dense in $L^2_{\mathbb{R}}(B, \mathrm{d}\mu)$.*

This is a pretty strange definition, and I will give some examples in a second, but let me first show how to use this definition to define what is meant by "local observables". Note that, thanks to the density condition above,

$$\mathcal{H}(B, \Omega) \stackrel{\mathrm{def}}{=} \mathcal{S}_B \times \mathcal{S}_B$$

is a symplectic subspace of $\mathcal{H}$ so that the restriction of $W_{\mathrm{F}} \circ z_\Omega$ to $\mathcal{H}(B, \Omega)$ is a representation of the CCR over $\mathcal{H}(B, \Omega)$.

Definition 2. *Let $\mathcal{K} = L^2_{\mathbb{R}}(K, \mathrm{d}\mu), \Omega, \mathcal{S}$ be as above and let B be a Borel subset of K. The algebra of local observables over B is the algebra*

$$\mathrm{CCR}_0(\mathcal{H}(B, \Omega)) = \text{span } \{W_{\mathrm{F}}(z_\Omega(Y)) \mid Y \in \mathcal{S}_B \times \mathcal{S}_B\}.$$

Note that Ω plays a role in the definition of $\mathcal{S}$ through the appearance of the spaces $\mathcal{K}_\lambda$. The first condition on $\mathcal{S}$ guarantees that $\mathcal{S} \times \mathcal{S} \subset \mathcal{H}$ so that, in particular, for all $Y \in \mathcal{S} \times \mathcal{S}$, $s(Y, \cdot)$ is well defined as a function on $\mathcal{H}$ which is important for the definition of the local observables to make sense. In practice, one wants to be able to use the same spatial structure $\mathcal{S}$ for various choices of Ω, in order to be able to compare different systems built over the same space $\mathcal{K} = L^2_{\mathbb{R}}(K, \mathrm{d}\mu)$. Note nevertheless that even then, the algebras of local and of quasi-local observables, which are algebras of bounded operators on the Fock space $\mathcal{F}^+(\mathcal{K}^{\mathbb{C}})$ do, *as sets*, depend on Ω. This is in contrast to the algebra of "all" observables,

$$\mathrm{CCR}_0(\mathcal{H}) = \text{span } \{W_{\mathrm{F}}(z_\Omega(Y)) \mid Y \in \mathcal{H}\} = \text{span } \{W_{\mathrm{F}}(\xi) \mid \xi \in \mathcal{K}^{\mathbb{C}}\},$$

which is, as a set, independent of Ω, as pointed out before. In other words, some of the physics is hidden in the way the local algebras are imbedded in the CCR algebra over $\mathcal{H}$.

4.3 Examples of local structures

Oscillator lattices – Klein-Gordon equations

In the case of the translationally invariant oscillator lattices in dimension 2 or higher presented in Sect. 2.2, $\mathcal{S}$ can be taken to be the space of sequences q of finite support, even in the massless case, as is easily checked. Alternatively, you could take $\mathcal{S}$ to be the larger space of sequences of fast decrease. This has

the advantage that then $\mathcal{S} \times \mathcal{S}$ is dynamics invariant. Note that in neither of these examples $\mathcal{S}\times\mathcal{S}$ is J invariant, though, so that $\mathcal{S}\times\mathcal{S}$ will not be a complex vector subspace of $(\mathcal{H}, J)$, just a real one. This is also true for $\mathcal{S}_B \times \mathcal{S}_B$ and will be crucial when discussing "local excitations of the vacuum" in quantum field theory.

Exercise 1. Check all of the above statements in detail.

As an example of a local observable, we have, with $\eta \in \mathcal{S}$ of bounded support in some set $B \subset \mathbb{Z}^d$,

$$\mathrm{e}^{\mathrm{i}\eta\cdot Q} = W_{\mathrm{F}}(\frac{\mathrm{i}}{\sqrt{2}}\Omega^{-1/2}\eta).$$

Very explicitly, one may think of taking $\eta(j) = \delta_{j,k}$ and then this is $\mathrm{e}^{\mathrm{i}Q(k)}$, a simple function of the displacement of the oscillator at site $k \in \mathbb{Z}^d$. At the risk of boring the wits out of you, let me point out yet again that this *fixed observable* is represented on Fock space by a *different operator* for different choices of Ω.

Similarly

$$\mathrm{e}^{\mathrm{i}\eta\cdot P} = W_{\mathrm{F}}(-\frac{1}{\sqrt{2}}\Omega^{1/2}\eta)$$

is a function of the momenta of the oscillators in the support of η.

In the one-dimensional translationally invariant lattice a spatial structure does not exist when $\nu = 1/2$ because of the strong infrared singularity. Indeed, due to the density condition in the definition of the local structure, it is clear that $\mathcal{S}$ must contain all sequences of finite support, and those do not belong to $\mathcal{K}_{-1/2}$ in dimension 1, as we already pointed out in Sect. 2.2.

Similarly, the wave and Klein-Gordon equations on $\mathbb{R}^d$ admit for example $C_0(\mathbb{R}^d)$ or the space of Schwartz functions as a spatial structure in dimension 2 or higher, as follows from the discussion in Sect. 2.2.

The finite dimensional case

I find this example personally most instructive. It forces one into an unusual point of view on a system of n coupled oscillators that is well suited to the infinite dimensional case. Think therefore of a system of n oscillators characterized by a positive n by n matrix Ω^2, as in Sect. 2.2. A local observable of such a system should be a function of the positions and momenta of a fixed finite set of oscillators. Does the definition given above correctly incorporate this intuition? Let's check.

In this case, $\mathcal{K} = \mathbb{R}^n$, which I view as $L^2_{\mathbb{R}}(K)$, where K is simply the set of n elements. Indeed, $q \in \mathbb{R}^n$ can be seen as a function $q : j \in \{1, \dots n\} \mapsto q(j) \in \mathbb{R}$, obviously square integrable for the counting measure. I already explained in detail the identification between the quantum state space $L^2(\mathbb{R}^n)$

and $\mathcal{F}^+(\mathbb{C}^n)$ (Sect. 3.3). Here $\mathbb{C}^n$ is the complexification of $\mathbb{R}^n$, and as such naturally identified with $L^2(K, \mathbb{C})$. So, finally

$$L^2(\mathbb{R}^n) \cong \mathcal{F}^+(L^2(K, \mathbb{C})).$$

Consider now a subset B of K, say $B = \{1, 6, 9\} (n \geq 9)$. It is an excellent exercise to convince oneself that, unraveling the various identifications, a local observable over B is a finite linear combination of operators on $L^2(\mathbb{R}^n)$ of the form $(a_j, b_j \in \mathbb{R}, j \in B)$:

$$\exp -\mathrm{i} \left(\sum_{j \in B} (a_j P_j - b_j Q_j) \right).$$

Better yet, if you write (with $\sharp B$ denoting the cardinality of the set B)

$$L^2(\mathbb{R}^n) \cong L^2(\mathbb{R}^{\sharp B}, \prod_{j \in B} \mathrm{d}x_j) \otimes L^2(\mathbb{R}^{n-\sharp B} \prod_{j \notin B} \mathrm{d}x_j),$$

then it is clear that the weak closure of the above algebra is

$$\mathcal{B}(L^2(\mathbb{R}^{\sharp B}, \prod_{j \in B} \mathrm{d}x_j)) \otimes \mathbb{1}.$$

So, indeed, a local observable is clearly one that involves only the degrees of freedom indexed by elements of B.

Exercise 2. Convince yourself all of this is true.

Unbounded local observables

To make contact with the physics literature, it will be convenient on occasion in the following to refer to polynomials in $\frac{\mathrm{d}}{\mathrm{d}t} W(z_\Omega(tY))|_{t=0}$ with $Y \in \mathcal{H}(B, \Omega)$ as local observables over B as well. These are sums of expressions of the form

$$\Pi_S(z_\Omega(Y_1))\Pi_S(z_\Omega(Y_2)) \ldots \Pi_S(z_\Omega(Y_n))$$

where each $Y_j \in \mathcal{H}(B, \Omega)$. Alternatively and perhaps more suggestively, these are sums of expressions of the form

$$(\eta_1 \cdot Q) \ldots (\eta_m \cdot Q) \quad \text{and} \quad (\eta_1 \cdot P) \ldots (\eta_m \cdot P),$$

or of products thereof, where each $\eta_j \in \mathcal{S}_B$. Again, for lattices, these are polynomials in the positions and momenta of the individual oscillators in some subset B of the lattice $\mathbb{Z}^d$.

4.4 Strictly localized vacuum excitations

I now want to give meaning to the notion of "local excitation of the vacuum" for general free oscillator fields with a local structure $\mathcal{S}$. So in this section $\mathcal{K} = L^2_{\mathrm{r}}(K, \mathrm{d}\mu)$, and $\mathcal{S}$ satisfies the conditions of Definition 1.

The equivalent classical notion is readily described and was already discussed in Sect. 2.2. The vacuum, being the ground state of the system, is the quantum mechanical equivalent of the global equilibrium $X = 0$, which belongs of course to the phase space $\mathcal{H}$, and a local perturbation of this equilibrium is an initial condition $X = (q, p) \in \mathcal{S} \times \mathcal{S}$ with the support of q and of p contained in a (typically bounded) subset B of K. An example of a local perturbation of an oscillator lattice is a state $X \in \mathcal{H}$ where only q_0 and p_0 differ from 0. In the classical theory, local perturbations of the equilibrium are therefore states that differ from the equilibrium state only inside a bounded subset B of K. It is this last formulation that is readily adapted to the quantum context, through the use of the notion of "local observable" introduced previously.

For that purpose, we first introduce the following notion, which is due to Knight [Kn].

Definition 3. *Let $\psi, \psi' \in \mathcal{F}^+(\mathcal{K}^{\mathbb{C}})$. We will say that ψ and ψ' are indistinguishable inside a Borel set $B \subset K$ if, for all $X \in \mathcal{H}(B, \Omega)$,*

$$\langle \psi | W_{\mathrm{F}}(z_\Omega(X)) | \psi \rangle = \langle \psi' | W_{\mathrm{F}}(z_\Omega(X)) | \psi' \rangle. \tag{44}$$

Note that, given ψ and B, it is easy to construct many states that are locally indistinguishable from ψ in B. Indeed, one may consider $W_{\mathrm{F}}(z_\Omega(X))|\psi\rangle$, for any $X \in \mathcal{H}(B^c, \Omega)$.

We are now ready to define what we mean by a strictly local excitation of the vacuum.

Definition 4. *If B is a Borel subset of K, a strictly local excitation of the vacuum with support in B is a normalized vector $\psi \in \mathcal{F}^+(\mathcal{K}^{\mathbb{C}})$, different from the vacuum itself, which is indistinguishable from the vacuum outside of B. In other words,*

$$\langle \psi | W_{\mathrm{F}}(z_\Omega(Y)) | \psi \rangle = \langle 0 | W_{\mathrm{F}}(z_\Omega(Y)) | 0 \rangle \tag{45}$$

for all $Y = (q, p) \in \mathcal{H}(B^c, \Omega)$.

For brevity, I will occasionally call such states "local states", although this terminology conjures up images that are misleading. In view of what precedes, the coherent states $W_{\mathrm{F}}(z_\Omega(X))|0\rangle$, for any $X \in \mathcal{H}(B, \Omega)$ are strictly local excitations of the vacuum in B. The use of the adjective "strictly" is motivated by the possibility of relaxing condition (45) to allow for states that are only approximately localized in B, but for which the expectation values of observables located far from B converge more or less rapidly to the corresponding vacuum expectation values. I refer to [DB2] for details.

4.5 Knight's theorem revisited

Recall that states with a finite number of field quanta, *i.e.* states belonging to $\mathcal{F}^{\mathrm{fin},+}(\mathcal{K}^{\mathbb{C}})$, are interpreted as states describing a finite number of quasi-particles (see Sect. 3.5). Hence one natural question is whether such a state can be a strictly local excitation of the vacuum in a set B. Theorem 1 below gives a necessary and sufficient condition for this to happen.

First, I need a definition:

Definition 5. *Ω is said to be strongly non-local on B if there does not exist a non-vanishing $h \in \mathcal{K}_{1/2}$ with the property that both h and Ωh vanish outside B.*

Here I used the further definition:

Definition 6. *Let $h \in \mathcal{K}_{\pm 1/2}$ and $B \subset K$. Then h is said to vanish in B if for all $\eta \in \mathcal{S}_B$, $\eta \cdot h = 0$. Similarly, it is said to vanish outside B, if for all $\eta \in \mathcal{S}_{B^c}$, $\eta \cdot h = 0$.*

Note that this definition uses the density of S_B in $L^2(B)$ implicitly, because without this property, it would not make much sense. Intuitively, a strongly non-local operator is one that does not leave the support of any function h invariant.

Theorem 1. *Let B be a Borel subset of K. Then the following are equivalent:*

(i) Ω is strongly non-local on B;

(ii) There do not *exist states in $\mathcal{F}^{fin,+}(\mathcal{K}^{\mathbb{C}})$ which are strictly strictly local excitations of the vacuum with support in $B \subset K$;*

I will give the proof of this result in Sect. 4.8.

Statement (i) of the theorem gives a more or less easily checked neccessary and sufficient condition for the non-existence of states with a finite number of field quanta that are localized in a region B. I will show in the examples developed in the following sections that this condition is so to speak always satisfied when B is a bounded set: I mean, it is satisfied in the various models that are typically studied in solid state physics, in relativistic quantum field theory, or in the theory of free quantum fields on curved space-times. Indeed, in these examples, Ω^2 is a finite difference or (second order elliptic) differential operator, so that it is local: it preserves the support. But its positive square root, Ω, is more like a pseudo-differential operator, and therefore does not preserve supports. This will be shown in several cases below. The upshot is that states with a finite number of particles, and a fortiori, one-particle states, are never strictly localized in a bounded set B. This gives a precise sense in which the elementary excitations of the vacuum in a bosonic field theory (relativistic or not) differ from the ordinary point particles of non-relativistic mechanics: their Hilbert space of states contains no states in which they are perfectly localized.

So, to sum it all up, you could put it this way. To the question

Why is there no sharp position observable for particles?

the answer is

It is the non-locality of Ω, stupid!

Should all this make you feel uncomfortable, I hope the further discussion in Sects. 4.7 of the history of the quest for a "position observable" in relativistic field theory will be of some help.

4.6 Examples

As a warm-up, here is my favourite example.

Exercise 3. Let $\mathcal{K} = \mathbb{R}^2$ so that Ω^2 is a two by two matrix and, as explained in Sect. 4.3, $K = \{1, 2\}$. Show that in this case, a state with a finite number of quanta can be a strictly localized excitation of the vacuum on $B = \{1\}$ only if Ω^2 is diagonal. In other words, this can happen only if the two oscillators are not coupled.

For typical translationally invariant systems, it is easy to see Ω is strongly non-local over bounded sets, so that we can conclude there are no strictly localized finite particle states. This is the content of the following results.

Theorem 2. *Let $\mathcal{K} = L^2_{\mathbb{R}}(\mathbb{R}^d, \mathrm{d}x)$ and let ω be a positive function belonging to $L^\infty_{\mathrm{loc}}(\mathbb{R}^d, \mathrm{d}k)$ with $\omega^{-1} \in L^1_{\mathrm{loc}}(\mathbb{R}^d, \mathrm{d}k)$. Suppose both ω and ω^{-1} are polynomially bounded at infinity. Let $\Omega = \omega(|\nabla|)$. Then $\mathcal{S} = \mathcal{S}(\mathbb{R}^d)$ is a local structure for this system. If ω does not extend to a holomorphic function on the complex plane, then Ω is strongly non-local on any bounded open set B. Consequently, there exist no states with a finite number of quasi-particles that are strictly localized excitations of the vacuum in such a set B.*

The proof is a simple application of the Paley-Wiener theorem together with Theorem 1. Note that the theorem applies to the Klein-Gordon equation: so we recover in this way Knight's original result. Pushing the use of the Paley-Wiener theorem a little further, one can also prove:

Theorem 3. *Let $\mathcal{K} = L^2_{\mathbb{R}}(\mathbb{R}^d, \mathrm{d}x)$ and $\Omega^2 = -\Delta + m^2$, with $d \geq 1, m > 0$, or $d \geq 2, m \geq 0$. Then $\mathcal{S} = \mathcal{S}(\mathbb{R}^d)$ is a local structure for this system and there exist no states with a finite number of quasi-particles that are strictly localized excitations of the vacuum in any set B with non-empty open complement.*

The result one needs here is proven in [SeGo]: for $\Omega = \sqrt{-\Delta + m^2}$, h and Ωh cannot both vanish on the same open set. Via Theorem 1 this implies the above result.

An analogous result holds for the translationally invariant lattices discussed in Sect. 2.2. In particular, with Ω^2 as in (10), it is very easy to see that there are no states with a finite number of quanta that are perfectly localized

perturbations of the vacuum on a finite number of lattice sites. The spatial structure is given here by the sequences of finite support, as discussed in Sect. 4.3.

Similarly, for the wave and Klein-Gordon equations the operator Ω is typically also strictly non-local, but I will not go into this here.

It is clear from these examples that Knight's theorem has less to do with relativity than with coupled oscillators, which is the point I wanted to make all along.

4.7 Newton-Wigner localization

Knight's result appears counterintuitive. Indeed, we argued first that the Fock space structure of the Hilbert space of states of the field invites a particle interpretation (Sect. 3.5), we then introduced what looks like a perfectly reasonable notion of "strictly localized excitation of the vacuum", only to end up discovering that states with a finite number of particles cannot be strictly localized. Since the notion of a particle evokes an entity that is localized in space, this may seem paradoxical. My point of view is simple: the way out of this paradox is, as I have suggested before (Sect. 3.5), that one has to keep in mind that the particles under discussion here are just *excited states of an extended system* and that, just like in an oscillator ring, chain, or lattice, the analogy with the point particles of elementary classical or quantum mechanics courses should not be pushed too far. Calling those excitations particles amounts to nothing more than an occasionally confusing abuse of language. The lesson to be learned from Knight's result is therefore that such field quanta may carry momentum and energy, but they cannot be perfectly localized. Viewed from the angle I have chosen, this is not even surprising. The examples showed indeed this statement is true in a system with two oscillators, and in oscillator lattices. One should in particular not hope to associate a position operator with those quanta, having all the usual properties familiar from the description of point particles in ordinary Schrödinger quantum mechanics.

I could end the story there. But a very different point of view, based precisely on the use of a position operator (the so-called Newton-Wigner position operator) to locate the particles, was developed well before Knight's work, in the context of (free) relativistic quantum field theory of which the Klein-Gordon field is a particular example. Since this alternative point of view has met with a certain amount of popularity, it cannot be dismissed too lightly. Below I will explain it has an obvious analog for the oscillator systems under study here and I will show why, although it seems at first sight perfectly natural, it is clearly ill-conceived. The implication of this remark for the debate about supposed causality problems in relativistic quantum field theory and a further overview of some other issues related to "particle localization" in that context will also be given.

Newton-Wigner localization: the definition

Let us therefore turn again to an oscillator field with spatial structure so that $\mathcal{K}^{\mathbb{C}} = L^2(K, \mathrm{d}\mu, \mathbb{C})$. The state space of this system is the bosonic Fock space $\mathcal{F}^+(\mathcal{K}^{\mathbb{C}})$ of which $\mathcal{K}^{\mathbb{C}} = L^2(K, \mathrm{d}\mu, \mathbb{C})$ represents the one-particle sector. Now, if the system is in the state $\psi \in \mathcal{K}^{\mathbb{C}} \subset \mathcal{F}^+(\mathcal{K}^{\mathbb{C}})$, it is in view of the particle interpretation of the field states explained in Sect. 3.5 very tempting to interpret $\mid \psi \mid^2 (y)\mathrm{d}\mu$ as the probability for finding the "particle" in a volume $\mathrm{d}\mu$ around y, or in a preciser manner, to say that the probability for finding the particle in $B \subset K$ is given by

$$\int_B \mid \psi \mid^2 (y)\mathrm{d}\mu.$$

This seems like a quite reasonable thing to do because it is completely analogous to what is done in the non-relativistic Schrödinger quantum mechanics of particle systems. I will call the projection valued measure $B \mapsto \chi_B$, where χ_B is the operator of multiplication by the characteristic function of B the Newton-Wigner position observable. If $\psi \in L^2(K, \mathrm{d}\mu, \mathbb{C})$ is supported in $B \subset K$, we say ψ is "Newton-Wigner localized in B". This terminology is inspired by the observation that, when considering the particular example of an oscillator field given by the wave or Klein-Gordon equation, one has $\mathcal{K} = L^2(\mathbb{R}^3, \mathrm{d}x, \mathbb{C})$ and in that case the above measure is indeed the joint spectral measure of the usual Newton-Wigner position operator of relativistic quantum field theory [NW]. This choice of position observable may seem reasonable, but it is only based on an analogy, and as I will now show, it is not reasonable at all.

For that purpose, let us go back to the particular example of the oscillator ring treated before (Sects. 2.2 and 4.3) and see what the Newton-Wigner position operator means in that case. Remember, this is just a system of n coupled oscillators. So the quantum Hilbert space can on the one hand be seen as $L^2(\mathbb{R}^n, \mathrm{d}x)$ (Schrödinger representation) and the system can be studied through the displacements and momenta of those oscillators. This is the usual point of view. Alternatively, it can be identified with the bosonic Fock space $\mathcal{F}^+(\mathcal{K}^{\mathbb{C}})$ (Fock representation), where now the one-particle subspace is $\mathcal{K}^{\mathbb{C}} = \mathbb{C}^n$. The latter, as explained in Sect. 4.3, can be thought of as $L^2(\mathbb{Z}/n\mathbb{Z}, \mathbb{C})$. In other words, it is tempting to interpret $\psi \in \mathcal{K}^{\mathbb{C}}$ as the quantum mechanical state of a "particle" hopping along n sites! Its probability of being at site i is then given by $|\psi(i)|^2$. More generally, any state of the n oscillators can be seen as a superposition of $0, 1, 2, \ldots$ "particle" states, where now "particle" refers to an imagined entity hopping along the sites of the chain. Speaking like this, we are pushing the particle interpretation maximally. The state $a^\dagger(\delta_i)|0\rangle$ is then thought of as particle perfectly localized on the site i.

But does this make sense? Certainly, whatever picture used, the mean square displacement of the oscillator at site j is a relevant physical observable in this system. The problem is that this mean square displacement will differ

from its vacuum value if $j \neq i$:

$$\langle 0|a(\delta_i)Q_j^2 a^\dagger(\delta_i)|0\rangle \neq \langle 0|Q_j^2|0\rangle.$$

So the idea that the system contains only one particle, and that the latter is localized perfectly at i, the rest of the sites being "empty", is not tenable. Indeed, if the particle is at site i, and if space (here represented by the n sites) is otherwise "empty", how can any observable at site j take a value different from its vacuum value? The problem is of course readily solved if one stops trying to interpret the quantity $|\psi(i)|^2$ as a probability of presence for a particle.

The same analysis carries immediately over to the oscillator chains or lattices discussed before. It is perhaps even more telling there. Now the one particle space is $\ell^2(\mathbb{Z}^d, \mathbb{C})$ and so the idea of thinking of states in this space as describing a particle hopping on the sites of the lattice $\mathbb{Z}^d$ may seem even more reasonable. Models of this type are used in solid state physics to describe lattice vibrations, and the quanta are then called phonons. They are excitations of the oscillator lattice and – as Knight's theorem tells us – cannot be perfectly localized in the sense that, if the system is in a one-phonon state $\psi \in \ell^2(\mathbb{Z}^d)$, then it cannot coincide with the vacuum outside a finite subset of the lattice. This does not lead to any interpretational difficulties, *as long as one does not try to interpret* $|\psi(i)|^2$ *as the probability of finding the particle at site* i *of the lattice.*

Finally, without any change whatsoever, the same analysis carries over to the Klein-Gordon equation. Let B be a bounded subset of $\mathbb{R}^3$ and $\psi \in L^2(\mathbb{R}^3, \mathrm{d}x, \mathbb{C})$ be supported in B. As Knight's theorem tells us, the corresponding one-particle state of the field is not an excitation of the vacuum localized inside B.

The conclusion I draw from all this is that *the Newton-Wigner operator does not provide an appropriate tool to describe the strict localization properties of the states of extended systems of the type discussed here.* It shows up only because of an understandable but ill-fated desire to force a *particle interpretation* with all its usual attributes on the states of a *field.* The right notion of a (strictly) localized state is the one given by Knight (Definition 4). This has lead to some debate in the context of relativistic quantum field theory, upon which I shall comment below. Anticipating on the discussion there, I would like to stress that my line of argument here, and in particular my criticism of the use of the Newton-Wigner operator has nothing to do with relativity, or with causality, but is related instead to the fact that we are dealing with extended systems.

Causality problems

In the early days of relativistic quantum field theory, and well before anything like Knight's theorem was formulated or proven, the particle interpretation

of the field states made it perfectly natural to search for a position operator with the usual properties familiar from non-relativistic quantum mechanics. In other words, if the field quanta are particles, one would want to answer the question: "Where is the particle?" It should therefore not come as a surprise that a fair amount of literature was devoted to this problem. The theory received its definite form in [NW] and a slightly more rigorous treatment was subsequently given in [Wi]. References to earlier work can be found in those two papers and in [ScWi]. The discussion in [NW] centers on the question how to identify, inside a relativistic elementary system (*i.e.* inside a unitary irreducible representation of the Poincaré group), a "position operator $\hat{x} = (\hat{x}_1, \hat{x}_2, \hat{x}_3)$", using only natural requirements – formulated as axioms – on the transformation properties of this operator under rotations and translations. The upshot of this analysis is that such an operator exists (for most values of spin and mass) and that it is unique. It is called the Newton-Wigner position operator in the literature. As an example, there exists such an operator in the one field quantum sector of the quantized Klein-Gordon field, which carries an irreducible representation of the Poincaré group of zero spin and it is precisely the one discussed in the previous subsection. Now, the joint spectral measure of the three components of $\hat{x}$ defines a projection valued measure P_B, where B is a Borel subset of $\mathbb{R}^3$. If the interpretation of $\hat{x}$ as a position operator along the lines of the usual interpretational rules of quantum mechanics is to make sense, then eigenstates of P_B with eigenvalue 1 are to be thought of as states "perfectly localized inside B". This is referred to as NW-localization. This is precisely the interpretation given to the Newton-Wigner operator in the literature which is, as explained before, at odds with Knight's notion of local excitation of the vacuum. Nevertheless, the axiomatic derivation of the Newton-Wigner operator, and its perfect analogy with the familiar situation in the quantum mechanics of non-relativistic particles gives it something very compelling, which probably explains its success. As a result, some authors have written that the Newton-Wigner operator is the only possible position operator for relativistic quantum particles. In [Wi], one reads the following claim: "I venture to say that any notion of localizability in three-dimensional space which does not satisfy [the axioms] will represent a radical departure from present physical ideas." Newton and Wigner say something similar, but do not put it so forcefully: "It seems to us that the above postulates are a reasonable expression for the localization of the system to the extent that one would naturally call a system unlocalizable if it should prove to be impossible to satisfy these requirements. In [ScWi] one can read: "One either accepts the Newton-Wigner position operator when it exists, or abandons his axioms. We believe the first alternative is well worth investigation and adopt it here." I of course have argued above that one should abandon it, and that this neither constitutes a departure from standard physical ideas, nor means that one abandons the notion of localizability.

Still, even among those that have advocated the use of Newton-Wigner localization, this notion has stirred up a fair amount of debate, since it violates causality, as I now briefly explain.

Indeed, first of all, a one-particle state of the Klein-Gordon field perfectly NW-localized in some bounded set B at an initial time, is easily seen to have a non-zero probability to be found arbitrarily far away from B, at any later time, violating causality. Since the theory is supposed to be relativistic, this is a real problem that has received much attention. Actually, replacing the projection operators P_B of the NW-position operator by any other positive operators transforming correctly under space translations, Hegerfeldt proved that the causality problem remains (see [He1] [He2] and for a more recent overview, [He3]). In addition, and directly linked to the previous observation, a state perfectly localized in one Lorentz frame is not in another one. These difficulties, while well known and widely stressed, are often dismissed with a vague appeal to one of the following somewhat related ideas. Although the Newton-Wigner derivation does not refer to any underlying field theory, these arguments all involve remembering that the "particles" in relativistic field theory are excitations of the field.

The first such argument goes as follows. In a field theory a position measurement of a particle would lead to pair creation (see [ScWi]) and so the appearance of particles far away is not paradoxical. This line of reasoning is not very satisfactory (as already pointed out in [NW]), since it seems to appeal to a (non-specified) theory of interacting fields to deal with the a priori simple non-interacting field. An alternative argument stresses that in a theory which allows for multi-particle states, the observation of exactly one particle inside a bounded set B entails the observation of the absence of particles everywhere else, and is therefore not really a local measurement. As such, the appearance later on of particles far away does not violate causality (see [Fu]). This argument is certainly correct. But it is again qualitative and nothing guarantees that it can correctly account for the "amount" of causality violation generated by the Newton-Wigner position.

All in all, it seems considerably simpler to adopt the notion of "strictly localized vacuum excitation" introduced by Knight, which is perfectly adapted to the study of the extended systems under consideration here and to accept once and for all that the particles of field theory are elementary excitations of the system (or field quanta) that do not have all the usual attributes of the point particles of our first mechanics and quantum mechanics courses. This seems to be the point of view implicitly prevalent among physicists, although it is never clearly spelled out in the theoretical physics textbooks for example, as I will discuss in more detail in [DB2]. It also has the advantage that no causality problems arise. Although traces of this argument can occasionally be found in the more mathematically oriented literature, Knight's definition of a strictly local excitation of the vacuum and his result on the non-localizability of finite particle states seem to be mostly ignored in discussions of the issue

of the localizability of particles in field theory, of which there continue to be many [Ba] [Ha] [Tel] [Stre] [Fl] [FlBu]

Having advocated Knight's definition of "local state", it remains to prove the extension of his theorem given above.

4.8 Proof of Theorem 1

The theorem is reduced to abstract nonsense through the following proposition. Note that, for any subset $\mathcal{M}$ of a Hilbert space $\mathcal{V}$, $\mathcal{M}^\perp$ denotes its orthogonal complement, which is a complex subspace of $\mathcal{V}$.

Proposition 2. *Let $\mathcal{K} = L^2_{\mathbb{R}}(K, \mathrm{d}\mu)$, Ω and $\mathcal{S}$ be as before. Let $B \subset K$. Then the following statements are equivalent.*

(i) Ω is strongly non-local over B.

(ii) $(z_\Omega(\mathcal{H}(B^c, \Omega)))^\perp = \{0\}$ or, equivalently,

$$(\overline{\mathrm{span}}_{\mathbb{C}} z_\Omega(\mathcal{H}(B^c, \Omega)))^\perp = \{0\}. \tag{46}$$

Indeed, that Theorem 1 (i) and (ii) are equivalent now follows from Theorem 4 below.

Proof. (Proposition 2) It is easy to see that $\xi \in (z_\Omega(\mathcal{H}(B^c, \Omega)))^\perp$ if and only if

$$\overline{\xi} \cdot \Omega^{1/2}\eta = 0 = \overline{\xi} \cdot \Omega^{-1/2}\eta,$$

for all $\eta \in \mathcal{S}_{B^c}$. We can suppose without loss of generality that ξ is real. Now, if $\xi \in \mathcal{K}$, then $\Omega^{1/2}\xi \in \mathcal{K}_{-1/2}$ and hence

$$0 = \xi \cdot \Omega^{1/2}\eta = \Omega^{1/2}\xi \cdot \eta$$

which proves $\Omega^{1/2}\xi$ vanishes outside B. Similarly $\Omega^{-1/2}\xi$ vanishes outside B. Setting $h = \Omega^{-1/2}\xi$ the result follows.

Theorem 4. *Let $\mathcal{W}$ be a real subspace of $\mathcal{V}$.*

(i) If $\psi \in \mathcal{F}^+((\overline{\mathrm{span}}_{\mathbb{C}}\mathcal{W})^\perp) \subset \mathcal{F}^+(\mathcal{V})$, $\| \psi \| = 1$, then

$$\langle \psi | W_{\mathrm{F}}(\xi) | \psi \rangle = \langle 0 | W_{\mathrm{F}}(\xi) | 0 \rangle, \qquad \forall \xi \in \mathcal{W}. \tag{47}$$

(ii) If $\mathrm{span}_{\mathbb{C}}\mathcal{W}$ is dense in $\mathcal{V}$ then there exist no $\psi \in \mathcal{F}^{\mathrm{fin},+}(\mathcal{V})$ other than $|0\rangle$ itself so that (47) holds.

Clearly, the equivalence of (i) and (ii) in Theorem 1 is obtained by taking $\mathcal{W} = z_\Omega(\mathcal{H}(B^{\mathrm{c}}, \Omega))$ in the above theorem and applying Proposition 2.

Proof. As a warm-up, let us prove that, if $|\psi\rangle = a^\dagger(\xi')|0\rangle$, for some $\xi' \in \mathcal{V}$, then (47) holds if and only if $\xi' \in (\overline{\mathrm{span}}_{\mathbb{C}}\mathcal{W})^\perp$ and $\| \xi' \| = 1$. Indeed, for all $\xi \in \mathcal{W}$,

$$\begin{aligned}\langle\psi|W_{\rm F}(\xi)|\psi\rangle &= \langle 0|a(\xi')[\mathbb{1}+a^\dagger(\xi)][\mathbb{1}-a(\xi)]a^\dagger(\xi')|0\rangle {\rm e}^{-\frac{1}{2}\|\xi\|^2}\\ &= \langle 0|W_{\rm F}(\xi)|0\rangle \parallel \xi' \parallel^2 -\langle 0|a(\xi')a^\dagger(\xi)a(\xi)a^\dagger(\xi')|0\rangle {\rm e}^{-\frac{1}{2}\|\xi\|^2}\\ &= \langle 0|W_{\rm F}(\xi)|0\rangle \left[\parallel \xi' \parallel^2 -(\overline{\xi}'\cdot\xi)(\overline{\xi}\cdot\xi')\right].\end{aligned}$$

Supposing (47) holds, this clearly implies $\parallel \xi' \parallel = 1$ and $\xi' \in (\overline{\rm span}_{\mathbb{C}}\mathcal{W})^\perp$. The converse is equally obvious. This proves the theorem for the very particular case of states containing exactly one quantum. Note that this completely characterizes the states with exactly one field quantum that are "localized".

To prove part (i), we can now proceed as follows. Recall that

$$W_{\rm F}(\xi) = {\rm e}^{-\frac{1}{2}\|\xi\|^2}{\rm e}^{a^\dagger(\xi)}{\rm e}^{-a(\xi)}.$$

Let $\xi \in \mathcal{W}$. Suppose $\psi = (\psi_0, \psi_1, \psi_2, \ldots, \psi_N, 0, 0, \ldots) \in \mathcal{F}^{\rm fin,+}((\overline{\rm span}_{\mathbb{C}}\mathcal{W})^\perp)$. Then

$$\langle\psi|W_{\rm F}(\xi)|\psi\rangle = {\rm e}^{-\frac{1}{2}\|\xi\|^2}\langle\psi,\psi\rangle = \langle 0|W_{\rm F}(\xi)|0\rangle.$$

Indeed, as a result of the fact that $\xi \in \mathcal{W}$ and $\psi \in \mathcal{F}^{\rm fin,+}((\overline{\rm span}_{\mathbb{C}}\mathcal{W})^\perp)$, it follows that $a(\xi)\psi = 0$ so that ${\rm e}^{-a(\xi)}\psi = \psi$. From this one can conclude as follows. For any $\psi = (\psi_0, \ldots, \psi_n, \ldots) \in \mathcal{F}^+((\overline{\rm span}_{\mathbb{C}}\mathcal{W})^\perp)$ and for any $N \in \mathbb{N}$, we can write

$$\psi = \psi_{<N} + \psi_{>N}$$

where $\psi_{<N} = (\psi_0, \ldots, \psi_N, 0, \ldots,)$. Then, for any $\epsilon > 0$, there exists $N_\epsilon \in \mathbb{N}$ so that

$$\langle\psi|W_{\rm F}(\xi)|\psi\rangle = \langle\psi_{<N_\epsilon}|W_{\rm F}(\xi)|\psi_{<N_\epsilon}\rangle + \mathcal{O}(\epsilon) = \langle 0|W_{\rm F}(\xi)|0\rangle + \mathcal{O}(\epsilon),$$

where the error term is uniform in ξ. Taking ϵ to 0, the result now follows.

In order to prove part (ii), I start with the following preliminary computation. Let $N \in \mathbb{N}$ and consider $\psi = (\psi_0, \psi_1, \psi_2, \ldots, \psi_N, 0, 0, \ldots) \in \mathcal{F}^{\rm fin,+}(\mathcal{V})$ with $\psi_N \neq 0$. We wish to compute, for any $t \in \mathbb{R}$, for any $\xi \in \mathcal{W}$,

$$\langle\psi|W_{\rm F}(t\xi)|\psi\rangle = \sum_{n,m=0}^{N}\langle\psi_n|W_{\rm F}(t\xi)|\psi_m\rangle.$$

We will first establish that

$$\langle\psi|W_{\rm F}(t\xi)|\psi\rangle{\rm e}^{\frac{1}{2}t^2\|\xi\|^2}$$

is a polynomial of degree at most $2N$ in t, for fixed ξ. For that purpose, it is enough to notice that any term of the type

$$\langle\psi_n|W_{\rm F}(t\xi)|\psi_m\rangle{\rm e}^{\frac{1}{2}t^2\|\xi\|^2}$$

is a polynomial of degree at most $n+m$. This follows from

$$\begin{aligned}\langle\psi_n|W_{\rm F}(t\xi)|\psi_m\rangle \mathrm{e}^{\frac{1}{2}t^2\|\xi\|^2} &= \langle\psi_n|\mathrm{e}^{a^\dagger(t\xi)}\mathrm{e}^{-a(t\xi)}|\psi_m\rangle \\ &= \sum_{\ell_1=0}^{n}\sum_{\ell_2=0}^{m}\frac{1}{\ell_1!\ell_2!}\langle\psi_n|(a^\dagger(t\xi))^{\ell_1}(-a(t\xi))^{\ell_2}|\psi_m\rangle\end{aligned}$$

It is clear that this is a polynomial of degree at most $n+m$. Also, the sum can actually be restricted to those ℓ_1, ℓ_2 for which

$$m-\ell_2 = n-\ell_1.$$

The term of degre $2N$ of the above polynomial is now easily identified:

$$\begin{aligned}\langle\psi_N|W_{\rm F}(t\xi)|\psi_N\rangle \mathrm{e}^{\frac{1}{2}\|t\xi\|^2} &= \langle\psi_N|\mathrm{e}^{a^\dagger(t\xi)}\mathrm{e}^{-a(t\xi)}|\psi_N\rangle \\ &= \sum_{\ell_1,\ell_2=0}^{N}\frac{1}{\ell_1!\ell_2!}\langle\psi_N|(a^\dagger(t\xi))^{\ell_1}(-a(t\xi))^{\ell_2}|\psi_N\rangle \\ &= \frac{(-1)^N t^{2N}}{N!N!}\langle\psi_N|(a^\dagger(\xi))^N(a(\xi))^N|\psi_N\rangle + \mathcal{O}(t^{2N-1}).\end{aligned}$$

Suppose now (47) holds for ψ. Then this polynomial actually has to be a constant, so, if $N \geq 1$,

$$(a(\xi))^N|\psi_N\rangle = 0$$

for all $\xi \in \mathcal{W}$. Now let $\xi_1 \ldots \xi_N \in \mathcal{W}$ and consider the polynomial

$$(a(t_1\xi_1 + \ldots + t_N\xi_N))^N|\psi_N\rangle = 0$$

in the variables $t_1, \ldots, t_N \in \mathbb{R}$. Since each of its coefficients must vanish, we conclude that

$$a(\xi_1)a(\xi_2)\ldots a(\xi_N)|\psi_N\rangle = 0,$$

for any choice of the $\xi_1 \ldots \xi_N \in \mathcal{W}$. Consequently, this is also true for any choice of $\xi_1 \ldots \xi_N \in \mathrm{span}_{\mathbb{C}}\mathcal{W}$. Introduce now an orthonormal basis η_i, $i \in \mathbb{N}$, of $\mathcal{V}$, with each $\eta_i \in \mathrm{span}_{\mathbb{C}}\mathcal{W}$. Then, in view of the above,

$$a(\eta_{\mathrm{i}_1})a(\eta_{\mathrm{i}_2})\ldots a(\eta_{\mathrm{i}_N})|\psi_N\rangle = 0,$$

for any choice $i_1 \ldots i_N \in \mathbb{N}$. It is then clear that $\psi_N = 0$. Since by hypothesis $\psi_N \neq 0$, it follows that $N = 0$, so that ψ belongs to the zero-particle subspace $\mathcal{F}_0^+(\mathcal{V})$.

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