The Quantization of Linear Dynamical Systems II: Infinite Systems

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This document begins (Section 1) by recalling its predecessor, *Quantization of Linear Dynamical Systems I*: which we call **Part I**. It was the pdf for 16 November 2021, presented on 15 Nov. 2021. It was mostly about systems with *finitely* many degrees of freedom. Taken together, the documents expound a rigorous quantization procedure developed by Irving Segal and others in the 1960s. This means we do not here cover algebraic quantum theory; which would emphasise topics like inequivalent representations, 'getting out of Fock space', Haag's theorem etc. (cf. e.g. Emch 1972); and which will be used in discussing e.g. the Unruh effect and elements of QFT on curved spacetimes.

The 'bottom-line' for the two documents taken together is that we have a procedure for quantizing (ie. constructing a representation of the Weyl algebra for) any of a special class of classical systems. The simple harmonic oscillator and the free real bosonic field both belong to this class; but of these two, only for the former (the finite system) does this construction pick out a unique representation.

We begin in Section 1 by recalling from Part I:

(i) quantization as the construction of a representation of the *Weyl algebra* associated with some classical system's phase space (endowed with suitable complex structure); and as "unitarizing" a Hamiltonian evolution in a symplectic space so as to give an evolution in a complex Hilbert space; cf. Sections 1-3 of Part I;

(ii) the ideas of a *one-particle structure* and of Fock space, i.e. symmetric Fock space built on any one-particle structure without regard to the details of dynamics; cf. Section 4 of Part I;

(iii) the Stone-von Neumann Theorem, which essentially guarantees that the quantization of the paradigm finite classical system, viz. point particles in $\mathbb{R}^n$, is unique (up to unitary equivalence); and its "fermionic cousin" the Jordan-Wigner theorem; cf. Section 6 of Part I.

Then we work up slowly to the free real bosonic Klein-Gordon field. We first look at two ways the premises of the Stone-von Neumann Theorem can fail: viz. with

(a) failure of weak continuity (Section 2);

(b) a classical configuration space other than $\mathbb{R}^n$, e.g. the circle S_1 (Section 3).

Then we look at an infinite spin chain, as an example where the premises of the Jordan-Wigner Theorem fail. This is an instructive system because one can easily show that unitary equivalence (of representations of the CARs) fails (Section 4).

Finally, section 5 focusses exclusively on the free real bosonic field, subject to the Klein-Gordon equation, and various interpretative issues, including particle localization and the interpretation of the local field operators $\Phi(\mathbf{x})$.

Contents

Sections 1 to 4 owe much to Chapters 2 and 3 of Ruetsche (2011). Section 5 is based on Baez *et al* (1992, Chapter 1) and Halvorson (2001).

1 Canonical quantization of finite systems: recalled

1.1 Quantization as representations of the Weyl algebra

(This summarises Section 1 of Part I.) A familiar way of developing elementary quantum mechanics is to "promote" the classical Poisson bracket relations

$$\{q^i, q^j\} = \{p_i, p_j\} = 0; \qquad \{q^i, p_j\} = \delta^i_j, \tag{1}$$

where $i, j \in \{1, 2, \ldots n\}$, to the *Heisenberg relations* (CCRs)

$$[Q^i, Q^j] = [P_i, P_j] = 0; \qquad [Q^i, P_j] = i\delta^i_j \mathbb{1}; \tag{2}$$

(where $\hbar := 1$) and to seek a representation of these quantities as self-adjoint operators on a Hilbert space. However, in hindsight, we know to expect the Q^is and P_js to have unbounded spectra, and therefore to not be fully defined on the space $L^2(\mathbb{R}^n)$ of square-integrable functions. This nuisance can be remedied by instead turning to the *Weyl form* of the CCRs.

Define, for any $\mathbf{a}, \mathbf{b} \in \mathbb{R}^n$,

$$U(\mathbf{a}) := e^{-i\mathbf{a}.\mathbf{P}}; \qquad V(\mathbf{b}) := e^{-i\mathbf{b}.\mathbf{Q}}; \tag{3}$$

Then, given (2), we have

$$U(\mathbf{a})V(\mathbf{b}) = e^{i\mathbf{a}.\mathbf{b}}V(\mathbf{b})U(\mathbf{a}). \tag{4}$$

Since the Us and Vs are both families of unitaries, their spectra are bounded, and are defined everywhere on $L^2(\mathbb{R}^n)$. We may take (4) as the primitive CCRs; our task is then to find representations of the Us and Vs.

But we are only halfway to our intended framing of the representation problem. Equation (4) can be given a more abstract presentation, which unifies the quantization of particles and bosonic fields. Setting $z := (\mathbf{a}, \mathbf{b}) \in \mathbb{R}^{2n}$, we define the family of operators

$$W(z) := e^{\frac{1}{2}i\mathbf{a}.\mathbf{b}}U(\mathbf{a})V(\mathbf{b}). \tag{5}$$

Then the Weyl form of the CCRs (4) are equivalent to the *Weyl algebra*

$$\begin{aligned} W(z_1)W(z_2) &= e^{\frac{1}{2}i\Omega(z_1,z_2)}W(z_1 + z_2); \\ W^\dagger(z) &= W(-z); \end{aligned} \tag{6}$$

for all $z, z_1, z_2 \in \mathbb{R}^{2n}$, where Ω is the *symplectic product*:

$$\Omega(z_1, z_2) := \mathbf{a}_2.\mathbf{b}_1 - \mathbf{a}_1.\mathbf{b}_2, \tag{7}$$

to be explained shortly. Importantly, the Weyl algebra (6), though abstract, may successfully be extended to bosonic fields.

1.2 Symplectic vector spaces and manifolds; linear systems

(This repeats from Part I: Section 3.3 and then part of Section 3.6.) If we are lucky enough for our classical phase space to be a vector space (as when $S = \mathbb{R}^{2n}$), then we can make it a *symplectic vector space*, which is a pair (S, Ω), where S is a phase space—also a vector space—and Ω is a symplectic product. The symplectic product $\Omega : S \times S \to \mathbb{R}$ is, by definition, anti-symmetric, linear and non-degenerate (i.e. if $\Omega(z_1, z_2) = 0$ for all z_2, then $z_1 = \mathbf{0}$).

We define the symplectic product on $S = \mathbb{R}^{2n} \ni z_1, z_2$ as in (7). Note that $\Omega(z, \cdot) : S \to \mathbb{R}$ is a real-valued function on S, and so a classical observable. In particular, $\Omega(z, \cdot) = q^i$ iff z has $(n+i)$th component $b_i = 1$ and the rest 0, and $\Omega(z, \cdot) = p_i$ iff z has ith component $a^i = -1$ and the rest 0. In general, $\Omega(z, \cdot)$ is some linear combination of p_is and q^is. In this formulation, the classical Poisson bracket relations (1) may be written

$$\{\Omega(z_1, \cdot), \Omega(z_2, \cdot)\} = -\Omega(z_1, z_2), \tag{8}$$

the corresponding Heisenberg form of the CCRs are

$$[\hat{\Omega}(z_1, \cdot), \hat{\Omega}(z_2, \cdot)] = -i\Omega(z_1, z_2)\mathbb{1}, \tag{9}$$

where (in the sought representation) the map $z \mapsto \hat{\Omega}(z, \cdot)$ takes elements of S to self-adjoint operators, and the Weyl unitaries are defined by

$$W(z) := e^{i\hat{\Omega}(z,\cdot)}. \tag{10}$$

This is Wald's presentation: see Wald (1994, Ch. 2). Later we will use field operators Φ, for which $\Phi(Jz) = \hat{\Omega}(z, \cdot)$, or $\Phi(z) = -\hat{\Omega}(Jz, \cdot) = \hat{\Omega}(\cdot, Jz)$.

Symplectic manifolds, more generally:— In the case where the classical phase space S is not a vector space, we must resort to a longer route. In this case, we seek a group whose action on S is *transitive* and preserves the symplectic form $\omega := \sum_i \mathrm{d}p_i \wedge \mathrm{d}q^i$. (In the case that S is a vector space, this group is just the (abelian) additive group of translations in S, which is isomorphic to S. That is what allowed us to treat S as a symplectic vector space above.) For illustration, taking the case $S = \mathbb{R}^{2n}$, the group action is a $2n$-parameter family of diffeomorphisms associated with the vector fields (with constant coefficients)

$$X_z = \sum_{i=1}^{n} b_i \frac{\partial}{\partial q^i} - a^i \frac{\partial}{\partial p_i}, \tag{11}$$

for any $z := (\mathbf{a}, \mathbf{b}) \in \mathbb{R}^{2n}$. We may now act on any two such vector fields with the *symplectic form* ω with which S, being a classical phase space, is equipped. This yields

$$\omega(X_{z_1}, X_{z_2}) = \mathbf{a}_2.\mathbf{b}_1 - \mathbf{a}_1.\mathbf{b}_2. \tag{12}$$

Our quantization problem then becomes the search for continuous families of unitaries $z \mapsto W(z)$ which respect this symplectic structure, as expressed in the Weyl algebra (6), setting $e^{\frac{1}{2}i\Omega(z_1,z_2)} = e^{\frac{1}{2}i\omega(X_{z_1},X_{z_2})}$. Since the Weyl algebra (6) is unitary up to the phase factor $e^{\frac{1}{2}i\omega(X_{z_1},X_{z_2})}$, it is a *projective unitary representation* of the group of symplectomorphisms on S.

Quadratic Hamiltonians and linear systems— We spell out how a Hamiltonian being quadratic implies that time-evolution preserves linear structure. So let the phase space Γ be a symplectic vector space with global coordinates (q, p). We write ξ^α, with α running from 1 to $2n$.

We now *define* a linear system as one in which the Hamiltonian is a quadratic form $H_{\alpha\beta}$ in the ξs. That is: the energy $= H = (\xi^\alpha)^T[H_{\alpha\beta}\xi^\beta]$. Then taking partial derivatives of the energy H with respect to any ξ^α (holding all other ξ^α constant of course) will give: a linear combination of the various ξ^β, i.e. a linear combination with constant coefficients. Call it $a_\alpha\xi^\alpha$ (with summation convention).Then ∇H is the column of these partial derivatives. Multiplying ∇H by the symplectic matrix keeps it a linear combination. So the Hamiltonian vector field is a linear combination of the various ξ^β with constant coefficients. Call it $b_\alpha\xi^\alpha$ (with summation convention).

So at each point $\xi = (q, p) \in \Gamma$, the infinitesimal flow is: $b_\alpha\xi^\alpha$. Then it is trivial that the time-evolution preserves the linear structure of solutions. For take two points: $\xi_1 = (q_1, p_1)$ and $\xi_2 = (q_2, p_2)$. At the sum-state got by superposing these states, $\xi_{1+2} := (q_1 + q_2, p_1 + p_2)$, the infinitesimal flow is by definition: $b_\alpha\xi^\alpha_{1+2}$. But this is: $b_\alpha(\xi^\alpha_1 + \xi^\alpha_2) = b_\alpha(\xi^\alpha_1) + b_\alpha(\xi^\alpha_2)$.

In short: The sum of two instantaneous states has as its infinitesimal Hamiltonian flow (tangent vector in phase space) the sum of the two states' individual Hamiltonian flows (tangent vectors).

1.3 One-particle structures

(This repeats passages of Section 4 (preamble and Section 4.2) from Part I.) There are two core ideas of the Segal quantization of a linear classical system.

First: there is a map K from the solution space of a classical linear system, i.e. a symplectic vector space, to a Hilbert space. K is required to satisfy conditions that combine the ideas of complex structures and symplectic structures, in such a way that the Hilbert space is determined. In short: we choose a complex structure J that preserves and tames the symplectic form, and we thereby complexify the real vector space and define a Hilbert space. Such a complex structure J is *not* unique. Besides, K is determined as having a unitary dynamics that is the "unitary cousin" of the classical system's dynamics. K, or the Hilbert space to which it leads, is called a *one-particle structure*.

Second: there is the usual Fock space construction, which will be applied to the one-particle structure's Hilbert space (i.e. after the first idea has been implemented). So here, the phrase 'one-particle' signals that the Hilbert space is the first (non-zero, i.e. non-vacuum) summand of the usual Fock space sum of ever larger tensor powers.

In Part I, we saw this illustrated for the harmonic oscillator (in one spatial dimension). Starting with classical harmonic oscillator, the first idea delivers us as the quantum state space— not the familiar quantum harmonic oscillator, with (in one spatial dimension) Hilbert space $L^2(\mathbb{R})$!—but 'merely' the world's simplest complex Hilbert space, viz. $\mathbb{C}$ i.e. the complex plane.

To get the familiar quantum harmonic oscillator, i.e. $L^2(\mathbb{R})$ (equipped with the quantum harmonic oscillator Hamiltonian), we need to take the Fock space built from $\mathbb{C}$. That Fock space will "be" (i.e. be a Hilbert space isomorphic to) $L^2(\mathbb{R})$. So we in effect *factorize* the usual understanding of canonical quantization—viz. (for the 1-dimensional harmonic oscillator) "replace the two-dimensional classical phase space $\mathbb{R}^2 \ni (q,p)$, with $L^2(\mathbb{R})$, i.e. L^2 functions on the configuration space $\mathbb{R}$—into: *first*, build a 1-particle structure; *second*, build the Fock space.

Here is a bit more detail about the first idea. (We postpone review of the second idea until later.)

We begin with the triple, $(\mathcal{S}, \Omega, \Phi_t)$, where $\mathcal{S}$ is a symplectic vector space, the 'phase/solution space' for a Hamiltonian system, Ω is its symplectic product, and Φ_t for the one-parameter group of motions (i.e. symplectomorphisms) along the integral curves of the Hamiltonian vector field X_h. We add a complex structure J that:

1. is a symplectomorphism; i.e. $\Omega(Jz_1, Jz_2) = \Omega(z_1, z_2)$ (it follows that $[J, \Phi_t] = 0$, i.e. J is equivariant under the classical dynamics);
2. "tames" Ω in that $\Omega(z, Jz) > 0$, for all $z \neq 0$.

Given this J, we define a complex inner product on (S, Ω, Φ_t, J):

$$\langle z_1, z_2 \rangle_{\mathcal{S}} := \frac{1}{2}\Omega(z_1, Jz_2) + \frac{1}{2}i\Omega(z_1, z_2), \tag{13}$$

Note: (This paragraph recalls the *Kahler condition*; cf. Sections 2.3.B to 2.3.D of Part I):—- The real part of this definition is using the idea that given a symplectic vector space V, with symplectic product ω, one can define a *complex-linear* but *real-valued* symmetric bilinear form g_J on the complex vector space V_J by: $g_J(u,v) := \omega(u, Jv)$. Then we use the idea that we can define a *sesquilinear*, *complex-valued* function on $V \times V$, i.e. complex inner product, in terms of g_J and ω, by: $\langle u, v \rangle \equiv \langle u, v \rangle_{\omega, J} := g_J(u,v) + i\omega(u,v)$.

1.4 The Stone-von Neumann and Jordan-Wigner uniqueness theorems

(This repeats passages of Section 6 from Part I.)

Theorem 1.1 (Stone-von Neumann Uniqueness Theorem)**.** *Let (S, Ω) be a symplectic vector space, with $S = \mathbb{R}^{2n}$. Every weakly continuous irreducible representation of the Weyl algebra over (S, Ω) is unitarily equivalent to the Schrödinger representation, in which, for all $\psi(\mathbf{x}) \in L^2(\mathbb{R}^n)$,*

$$(W(\mathbf{a}, \mathbf{b})\psi)(\mathbf{x}) := e^{-i\mathbf{a}.(\mathbf{x} - \frac{1}{2}\mathbf{b})}\psi(\mathbf{x} - \mathbf{b}). \tag{14}$$

Note as special cases that $(W(\mathbf{a}, \mathbf{0})\psi)(\mathbf{x}) \equiv (U(\mathbf{a})\psi)(\mathbf{x}) = \psi(\mathbf{x} - \mathbf{a})$ and $(W(\mathbf{0}, \mathbf{b})\psi)(\mathbf{x}) \equiv (V(\mathbf{b})\psi)(\mathbf{x}) = e^{-i\mathbf{b}.\mathbf{x}}\psi(\mathbf{x})$. In fact, the Schrödinger representation is strongly continuous. So by Stone's Theorem, there are $2n$ self-adjoint operators, Q^i and P_i, such that $U(\mathbf{a}) = e^{-i\mathbf{a}.\mathbf{P}}$, $V(\mathbf{b}) = e^{-i\mathbf{b}.\mathbf{Q}}$ and for all $\psi(\mathbf{x}) \in L^2(\mathbb{R}^n)$ in suitable domains,

$$(\mathbf{Q}\psi)(\mathbf{x}) = \mathbf{x}\psi(\mathbf{x}); \qquad (\mathbf{P}\psi)(\mathbf{x}) = -i\nabla\psi(\mathbf{x}). \tag{15}$$

For the Jordan-Wigner theorem for the CARs, we consider first a sequence of quantum theories, each corresponding to a chain of spin-$\frac{1}{2}$ systems. The first theory describes a single spin-$\frac{1}{2}$ system, with observables $\{\sigma(x), \sigma(y), \sigma(z)\}$, which satisfy the Pauli relations

$$[\sigma(x), \sigma(y)] = 2i\sigma(z) \quad \text{and cyclic perms}; \qquad \sigma^2 := \sigma(x)^2 + \sigma(y)^2 + \sigma(z)^2 = 3\mathbb{1}. \tag{16}$$

This is equivalent to satisfying the canonical *anti*-commutation relations (CARs; see e.g. pp. 60-61 of Ruetsche 2011),

$$d^2 = \left(d^\dagger\right)^2 = 0; \qquad [d, d^\dagger]_+ = 1; \tag{17}$$

where

$$\sigma(x) = d + d^\dagger; \quad \sigma(y) = -i\left(d - d^\dagger\right); \quad \sigma(z) = dd^\dagger - d^\dagger d. \tag{18}$$

We now consider a theory describing a linear chains of n spin-$\frac{1}{2}$ systems, with observables $\{\sigma_k(x), \sigma_k(y), \sigma_k(z) \mid k \in \{1, 2, \ldots n\}\}$, satisfying

$$[\sigma_j(x), \sigma_k(y)] = 2i\delta_{jk}\sigma_k(z) \quad \text{and cyclic perms;} \qquad \sigma_k^2 := \sigma_k(x)^2 + \sigma_k(y)^2 + \sigma_k(z)^2 = 3\mathbb{1}. \tag{19}$$

Of course, our theory falls outside the scope of the Stone-von Neumann theorem, because it is characterized by CARs, rather than CCRs. However, there is an analogous uniqueness theorem:

Theorem 1.2 (Jordan-Wigner Uniqueness Theorem)**.** *For each finite n, every irreducible representation of the CARs (equivalently, the Pauli relations) is unitarily equivalent to the Pauli representation, in which*

$$\begin{aligned}
\sigma_k^P(x) &= \underbrace{\mathbb{1} \otimes \ldots \otimes \mathbb{1}}_{k-1} \otimes \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \otimes \underbrace{\mathbb{1} \otimes \ldots \otimes \mathbb{1}}_{n-k}; \\
\sigma_k^P(y) &= \underbrace{\mathbb{1} \otimes \ldots \otimes \mathbb{1}}_{k-1} \otimes \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \otimes \underbrace{\mathbb{1} \otimes \ldots \otimes \mathbb{1}}_{n-k}; \\
\sigma_k^P(z) &= \underbrace{\mathbb{1} \otimes \ldots \otimes \mathbb{1}}_{k-1} \otimes \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \otimes \underbrace{\mathbb{1} \otimes \ldots \otimes \mathbb{1}}_{n-k}.
\end{aligned} \tag{20}$$

The Stone-von Neumann theorem fails to apply if either of its antecedent conditions fail; i.e. if either the classical phase space is not $\mathbb{R}^{2n}$, or else the representation of the Weyl algebra is not weakly continuous. Following Ruetsche (2011, Ch. 3), it is helpful to break the various possible failures into three cases:

(i) weak continuity fails;

(ii) classical phase space is finite-dimensional, but not $\mathbb{R}^{2n}$;

(iii) classical phase space is infinite-dimensional.

In each of these cases, we have no guarantee that the quantization of our classical system is unique. In fact, for each of these cases we know that the quantization is not unique.

We will investigate case (i) in Section 2, case (ii) in Section 3, and case (iii) in Section 5. But before case (iii), we will deal (in Section 4) with infinite spin chains, i.e. with the break-down analogous to case (iii) for CARs.

2 Dropping weak continuity—and getting position or momentum eigenstates

There are representations of the CCRs that give up weak continuity (aka: regularity) whose Hilbert space contains exact position eigenstates: but these are not the "improper eigenstates" given by delta-functions (cf. our Hilbert space Review), nor the eigenstates of "rigged Hilbert space". By a parallel construction, one can build a non-regular representation with exact momentum eigenstates. To explain this, we will follow Halvorson, "Complementarity of representations in quantum mechanics", *Studies in History and Philosophy of Modern Physics* 2004.

His paper develops results from the 1970s, e.g. by Beaume et al. A philosophers' review of Halvorson is in Ruetsche 2011, Chapter 3.1.

These constructions are of interest for several reasons:—

(i) They use a *non-separable Hilbert space*: a kind of quantum state-space relevant to various foundational/interpretative discussions (reviewed by Earman, "Quantum Physics in Non-separable Hilbert spaces", Pittsburgh archive 2020: Earman's Section 5.2 discusses this case).

(ii) In the representation with exact position eigenstates, there are no momentum eigenstates; indeed, the momentum operator *does not exist*. And vice versa: the representation with exact momentum eigenstates has no position eigenstates, and no position operator. Besides, these representations are unitarily *inequivalent*. (Non-separable Hilbert spaces and unitarily inequivalent representations will be themes for us below.)

(iii) Building on (ii), Halvorson sees these results as formulating (vindicating!) Bohr's doctrine of complementarity (this theme is also in other contemporary papers of his). We recall from our Hilbert space Review, that in $L^2(\mathbb{R})$, complementarity is usually taken to be formulated by such facts as:

(a) the position-momentum uncertainty relation (i.e. the product of the standard deviations of any function and its Fourier transform is lower bounded); and

(b) the meet of (intersection of the ranges of) any compact-support spectral projector for position with any compact-support spectral projector for momentum is the zero projector (subspace); (cf.: for any function of bounded support, its Fourier transform has unbounded support).

Whether or not Bohr (or we!) really "want" a quantum particle to be able to have a precise/sharp *real-number* position, or momentum—but not both!—in a way that goes beyond (a) and (b) . . . is a matter for discussion! This is taken up by Ruetsche ibid. and e.g.: B Feintzeig et al. Why be regular? Part I, *Studies in History and Philosophy of Modern Physics* 2019; and B Feintzeig and J Weatherall, Why be regular? Part II, *Studies in History and Philosophy of Modern Physics* 2019; and B Feintzeig, The classical limit of a state on the Weyl algebra, *Journal of Mathematical Physics* 2018.

We now construct a representation with position eigenstates, guided by the familiar Schrödinger representation. (Then, *mutatis mutandis*, we will build a momentum representation.) But unlike the familiar case, our representation will be carried by the non-separable Hilbert space $l^2(\mathbb{R})$ of all square-summable functions $\psi : \mathbb{R} \to \mathbb{C}$. These are functions ψ supported on a *countable* set of real numbers, $\sigma(\psi) \subset \mathbb{R}$, and that satisfy

$$||\psi||^2 := \sum_{x \in \sigma(\psi)} |\psi(x)|^2 < \infty \, . \tag{21}$$

Here $||\psi||$ is the norm derived from the inner product $\langle \psi, \phi \rangle = \sum_{x \in \sigma(\psi) \cap \sigma(\phi)} \psi^*(x)\phi(x)$. The space $l^2(\mathbb{R})$ is spanned by the continuum-many states (characteristic functions of real numbers)

$$\psi_\lambda(x) = \begin{cases} 1 & \text{if} \quad x = \lambda, \\ 0 & \text{if} \quad x \neq \lambda. \end{cases} \tag{22}$$

The $\{\psi_\lambda : \lambda \in \mathbb{R}\}$ are an orthonormal basis of $l^2(\mathbb{R})$.

We define the representations of the Weyl unitaries using these basis states, and guided by the Schrödinger representation. We define for each $a, b \in \mathbb{R}$:

$$(U(a)\psi_\lambda)(x) := \psi_\lambda(x - a) \equiv \psi_{\lambda+a}(x); \qquad (V(b)\psi_\lambda)(x) := e^{-ibx}\psi_\lambda(x) \equiv e^{-ib\lambda}\psi_\lambda(x). \tag{23}$$

Since for each $a, b \in \mathbb{R}$, $U(a)$ and $V(b)$ map an orthonormal basis to another, they extend to unitaries. One checks that the Weyl relations, eq. 4, hold.

It can now be checked that weak continuity fails for the Us. Recall (from Section 6.1 of Part I) that weak continuity requires that for every vector ψ in the Hilbert space, $\langle\psi, U(a+\varepsilon)\psi\rangle \to \langle\psi, U(a)\psi\rangle$ as $\varepsilon \to 0$. Then we note that

$$\langle\psi_\lambda, U(a)\psi_\lambda\rangle = \begin{cases} 1 & \text{if} \quad a = 0, \\ 0 & \text{if} \quad a \neq 0, \end{cases} \tag{24}$$

and so $U(a)$ is not weakly continuous at $a = 0$. It follows that Stone's Theorem (cf. Section 3.6 of Hilbert space Review) does not apply, and we have no self-adjoint operator, the would-be momentum, to generate spatial translations. More precisely: Stone's theorem does not apply, so that we cannot define the momentum operator in the standard way by taking the derivative $-i(dU(a)/da)|_{a=0}$. (For discussion of a more general conception of "having a momentum operator", cf. e.g. Halvorson 2004, Section 4.)

Note that Stone's theorem is often formulated with an assumption of strong continuity on the 1-parameter group (e.g. De Faria and De Melo, 2010, Appendix A.9, p. 250). But in fact for 1-parameter unitary groups, weak continuity implies strong continuity; (by a simple argument, e.g. Prugovecki 2006, Lemma 6.2, p. 234).

On the other hand, the Vs are weakly continuous. For trivially, on our orthonormal basis, for any $\lambda \in \mathbb{R}$: $\langle\psi_\lambda, V(b)\psi_\lambda\rangle \equiv e^{ib\lambda} \to 1$ as $b \to 0$. So the Vs are weakly continuous, and therefore also strongly continuous; and so by Stone's Theorem, there is a self-adjoint operator Q such that $V(b) = e^{ibQ}$. Its action on our orthonormal basis is as we want:

$$(Q\psi_\lambda)(x) = -i \lim_{b\to 0} b^{-1}(V(b) - I)\psi_\lambda(x) = -i \lim_{b\to 0} b^{-1}(e^{ib\lambda} - I)\psi_\lambda(x) = \lambda\psi_\lambda(x). \tag{25}$$

So much by way of constructing a position representation. Alternatively, we can *mutatis mutandis* build a momentum representation on $l^2(\mathbb{R})$. The situation is then reversed: the Vs fail to be weakly continuous, and so fail to yield a self-adjoint generator, the would-be position operator; while the Us are generated by a momentum operator satisfying the expected eigenvalue equation.

These two representations on $l^2(\mathbb{R})$, the position and momentum representations, are not unitarily equivalent. This can be seen immediately: no unitary A exists such that $AQA^\dagger$, with Q as defined in (25), is the position operator in the momentum representation—for no such operator exists!

3 Nontrivial configuration spaces: a particle on the circle

For a particle on the circle, the configuration space is S^1, coordinatized by $\phi \in [0, 2\pi)$ and the phase space is $S = S^1 \times \mathbb{R}$, coordinatized by $(\phi, l) \in [0, 2\pi) \times \mathbb{R}$. This phase space cannot be a symplectic vector space, since S^1 is not a vector space. But it is a symplectic manifold, with symplectic form $\omega = \mathrm{d}l \wedge \mathrm{d}\phi$. Therefore we have to look for the group of symplectomorphisms on S. This is a 2-parameter family, generated by the vector fields

$$X_z = b\frac{\partial}{\partial\phi} - a\frac{\partial}{\partial l}, \tag{26}$$

where $z := (a, b) \in \mathbb{R}^2$. As discussed in Section 3 of Part I, this parameter space can be given the structure of a symplectic manifold by defining

$$\Omega(z_1, z_2) := \omega(X_{z_1}, X_{z_2}) = a_2 b_1 - a_1 b_2. \tag{27}$$

Inspired by the Schrödinger representation on $L^2(\mathbb{R})$, we might want to define the Weyl unitaries on $L^2(S^1) \ni \psi(\phi)$, according to:

$$(V(b)\psi)(\phi) := e^{-ib\phi}\psi(\phi); \qquad (U(a)\psi)(\phi) := \psi(\phi - a). \tag{28}$$

But now we face the problem that ψ is only defined on $[0, 2\pi)$, while a may be any real number. The standard solution (see Morandi 1992, Ch. 3) is to seek representations not in the space of square-integrable functions on S^1, but rather on its *universal covering space*, $\mathbb{R}$, coordinatized by $\tilde{\phi}$. The idea is that a phase θ is picked up for each 2π translation along $\mathbb{R}$; and different choices of θ give unitarily inequivalent representations of the Weyl relations.

In detail:— The group $\pi_1(S^1)$ of homotopy equivalence classes $[\gamma]$ on S^1 (where γ is a loop on S^1) acts on the real line in the obvious way. Note that $\pi_1(S^1) \cong \mathbb{Z}$. Namely: if $[k]$ is the class of loops circling S^1 $|k|$ times, clockwise if $k > 0$ and anti-clockwise if $k < 0$ (so $k \in \mathbb{Z}$), then the action is: $[k] \cdot \tilde{\phi} := \tilde{\phi} + 2\pi k$. Given this action, we require the states $\tilde{\psi} \in L^2(\mathbb{R})$ to satisfy the condition

$$\tilde{\psi}([\gamma] \cdot \tilde{\phi}) = a([\gamma])\tilde{\psi}(\tilde{\phi}), \tag{29}$$

where $a : \pi_1(S^1) \to U(1)$ is a 1-dimensional unitary representation of $\pi_1(S^1)$.

Let $[+1]$ be the class of loops circling S^1 once clockwise, and let $a([+1]) =: e^{i\theta}$, where $\theta \in [0, 2\pi)$. Here we see how the choice of the representation a fixes the phase picked up by a single translation by 2π—and thus by any integer number of such translations. That is: this implies that $a([k]) = e^{ik\theta}$, where $k \in \mathbb{Z}$. It then follows, using eq. 28 and 29, that

$$(U(2k\pi)\tilde{\psi})(\tilde{\phi}) = e^{-ik\theta}\tilde{\psi}(\tilde{\phi}) \ . \tag{30}$$

It may be checked that

$$(V(b)\tilde{\psi})(\tilde{\phi}) := e^{-ib\tilde{\phi}}\tilde{\psi}(\tilde{\phi}); \qquad (U_\theta(a)\tilde{\psi})(\tilde{\phi}) = e^{-i\frac{a\theta}{2\pi}}\tilde{\psi}(\tilde{\phi} - a); \tag{31}$$

satisfy the required Weyl relations and condition (30).

The self-adjoint generator of the U_θs is the angular momentum operator

$$L_\theta = -i\frac{\mathrm{d}}{\mathrm{d}\tilde{\phi}} + \frac{\theta}{2\pi}, \tag{32}$$

which, due to (30), has the discrete spectrum $\{k + \frac{\theta}{2\pi} \mid k \in \mathbb{Z}\}$.

Since the spectra of any two $L_{\theta_1}, L_{\theta_2}$, where $\theta_1 \neq \theta_2$, are disjoint, no two representations are unitarily equivalent.

But the value of θ has empirical consequences, as illustrated by the related examples: (i) the Aharonov-Bohm effect; and (ii) anyons. In both of these cases the configuration space's first homotopy group is $\pi_1(\mathcal{Q}) \cong \mathbb{Z}$, like the particle on the circle.

4 Infinite degrees of freedom 1: the infinite spin chain

Recall Section 1.4 above about the Jordan-Wigner theorem, and its specification of the Pauli representation (which we labelled 'P') on a *finite* spin chain: which recalled Section 6.1 of **Part I**. We now **repeat** more of that Section 6.1.

An alternative to the Pauli representation (though, by the Jordan-Wigner theorem, equivalent to it) is the representation S ('S' for 'switch') that defines the spin matrices according to

$$\sigma_k^S(x) = \sigma_k^P(y); \qquad \sigma_k^S(y) = \sigma_k^P(z); \qquad \sigma_k^S(z) = \sigma_k^P(x); \qquad k = 1, 2, ..., n \tag{33}$$

i.e. the switch representation of $\sigma_k(x)$ in $\mathcal{H}_S$ has the same matrix elements as the Pauli representation of $\sigma_k(y)$ in $\mathcal{H}_P$, etc. Now let $U : \mathbb{C}^2_P \to \mathbb{C}^2_S$ be the unitary such that $U\sigma^P(y)U^\dagger = \sigma^S(x)$, etc. Then the unitary $\otimes^n U : \mathcal{H}_P \to \mathcal{H}_S$ (with $\mathcal{H}_P \equiv \mathbb{C}^{2n}$) establishes the unitary equivalence between the switch and Pauli representations.

This equivalence extends to all operators in $\mathcal{B}(\mathcal{H}_S)$ and $\mathcal{B}(\mathcal{H}_P)$. In particular, let $\{f_i(\{\sigma_k^P(u_i)\})\}$ be a sequence of linear functions of the $\{\sigma_k^P(u_i)\}$ which converges in $\mathcal{H}_P$'s weak topology to the operator F_P. Here, for each i, u_i is one of the three coordinate labels, x, y, z. Each $f_i(\{\sigma_k^P(u_i)\}) \in \mathcal{B}(\mathcal{H}_P)$ and $\mathcal{B}(\mathcal{H}_P)$ is closed under weak convergence; so $F_P \in \mathcal{B}(\mathcal{H}_P)$. Similarly, let $\{f_i(\{\sigma_k^S(u_i)\})\}$ be a sequence of linear functions of the $\{\sigma_k^S(u_i)\}$, where

$$f_i(\{\sigma_k^S(u_i)\}) = U f_i(\{\sigma_k^P(u_i)\}) U^\dagger. \tag{34}$$

Weak convergence is preserved under unitary transformations, so the $\{f_i(\{\sigma_k^S(u_i)\})\}$ converge in $\mathcal{H}_S$'s weak topology to some operator $F_S \in \mathcal{B}(\mathcal{H}_S)$, and $F_S = U F_P U^\dagger$.

In the Pauli representation $\mathcal{H}_P \cong \mathbb{C}^{2n}$, we may define the *polarization* observable (a vector quantity) $\hat{\mathbf{m}}^P := (m_x^P, m_y^P, m_z^P)$, where

$$m_x^P := \frac{1}{n} \sum_{k=1}^{n} \sigma_k^P(x), \quad \text{etc.} \tag{35}$$

Clearly, $\hat{\mathbf{m}}^P \in \mathcal{B}(\mathcal{H}_P)$. That is, each of its three components $\in \mathcal{B}(\mathcal{H}_P)$. And the spectrum of $\hat{\mathbf{m}}^P$ is parameterized by points on the unit sphere. From the above considerations, we know that the similarly defined polarization observable $\hat{\mathbf{m}}^S := (m_x^S, m_y^S, m_z^S)$ in the switch representation satisfies

$$\hat{\mathbf{m}}^S = U \hat{\mathbf{m}}^P U^\dagger, \tag{36}$$

and so expectation values in the representation S are identical to corresponding (given U) expectation values in the representation P.

Now consider the theory of the *infinite spin-chain*, in which we have a spin-$\frac{1}{2}$ system for every integer in $\mathbb{Z}$. This theory has observables satisfying the Pauli relations (19). Representations of the Pauli relations in such a theory will be carried by a separable Hilbert space only if we make some hard choices about which of the uncountably many *prima facie* possible states are to be excluded.

(References for what follows include, G. Sewell's books, *Quantum Theory of Collective Phenomena* 1986, and *Quantum Mechanics and its Emergent Macrophysics* 2002; cf. Section 2.3 of each book. The natural proposal to set $\mathcal{H}$ = the infinite tensor product of $\mathbb{C}^2$ leads to a non-separable Hilbert space, since it has $2^{\aleph_0}$ dimensions: cf. Section 2.1 of Earman, "Quantum Physics in Non-separable Hilbert spaces", Pittsburgh archive 2020.)

One way to construct a separable Hilbert space is to pick a single-site state-vector $|\theta, \phi\rangle$ that we favour. Let $|\theta, \phi\rangle$ be the eigenstate (with eigenvalue 1) for the spin vector's being $\hat{\mathbf{u}}_{(\theta,\phi)}$: which latter is the unit vector intersecting the unit sphere at latitude $\frac{\pi}{2} - \theta$ and longitude ϕ. Our Hilbert space $\mathcal{H}_{(\theta,\phi)}$ is then constructed as follows. First, it contains the state in which *every* spin-site has state $|\theta, \phi\rangle$; call this state $\Omega_{(\theta,\phi)}$. Then we generate $\mathcal{H}_{(\theta,\phi)}$ by taking the closed linear span of all states obtained from $\Omega_{(\theta,\phi)}$ by $SU(2)$ rotations on any *finite* number of the spin sites.

We can do this as follows. (Cf. the definitions of the operators d in eq. 17 and 18 of Section 1.4.) First: define $\mathcal{H}_{(\theta,\phi)}$ as a fermionic Fock space on $l^2(\mathbb{Z})$:

$$\mathcal{H}_{(\theta,\phi)} := \mathfrak{F}_- \left[l^2(\mathbb{Z}) \right] = \mathbb{C} \oplus l^2(\mathbb{Z}) \oplus \mathcal{A}_2 \left[l^2(\mathbb{Z}) \otimes l^2(\mathbb{Z}) \right] \oplus \dots \tag{37}$$

The subspace $\mathcal{A}_N \left[\otimes^N l^2(\mathbb{Z}) \right]$ corresponds to arbitrary superpositions of states in which exactly N spin sites are in an eigenstate of pointing in the direction $-\hat{\mathbf{u}}_{(\theta,\phi)} \equiv \hat{\mathbf{u}}_{(\pi-\theta,\phi+\pi)}$ and all remaining spin sites are in an eigenstate of pointing in the familiar direction $\hat{\mathbf{u}}_{(\theta,\phi)}$.

We define the "vacuum" state $\Omega_{(\theta,\phi)}$ by

$$\Omega_{(\theta,\phi)} = 1 \oplus \mathbf{0} \oplus \mathbf{0} \oplus \ldots \tag{38}$$

We now define fermionic creation and annihilation operators $d_k^\dagger, d_k$ for each spin site $k \in \mathbb{Z}$. $\mathcal{H}_{(\theta,\phi)}$ is the closed linear span of arbitrary combinations of these acting on $\Omega_{(\theta,\phi)}$. First we define the operators ${d_k^{(N)}}^\dagger : \otimes^{N-1} l^2(\mathbb{Z}) \to \otimes^N l^2(\mathbb{Z})$ and $d_k^{(N)} : \otimes^N l^2(\mathbb{Z}) \to \otimes^{N-1} l^2(\mathbb{Z})$ for all $N \in \mathbb{N}$:

$$\begin{array}{rcl} {d_k^{(N)}}^\dagger (\psi_1 \otimes \ldots \otimes \psi_{N-1}) & := & \chi_k \otimes \psi_1 \otimes \ldots \otimes \psi_{N-1} \\ d_k^{(N)} (\psi_1 \otimes \psi_2 \otimes \ldots \otimes \psi_N) & := & \psi_1(k)\ \psi_2 \otimes \ldots \otimes \psi_N \end{array} \tag{39}$$

where $\chi_k(j) = \delta_{jk}$. Now we may define $d_k^\dagger, d_k : \mathfrak{F}_- \left[l^2(\mathbb{Z})\right] \to \mathfrak{F}_- \left[l^2(\mathbb{Z})\right]$ by

$$\begin{array}{rcccccccc} {d_k}^\dagger & := & {d_k^{(1)}}^\dagger & \oplus & \sqrt{2}\mathcal{A}_2 {d_k^{(2)}}^\dagger & \oplus & \sqrt{3}\mathcal{A}_3 {d_k^{(3)}}^\dagger & \oplus & \ldots \\ d_k & := & 0 & \oplus & d_k^{(1)} & \oplus & \sqrt{2} d_k^{(2)} & \oplus & \sqrt{3} d_k^{(3)} \oplus \ldots \end{array} \tag{40}$$

It may be checked that

$$[d_j, d_k]_+ = [d_j^\dagger, d_k^\dagger]_+ = 0; \qquad [d_j, d_k^\dagger]_+ = \delta_{jk}\ . \tag{41}$$

We may now define

$$\begin{array}{rcl} \sigma_k^{(\theta,\phi)}(x) & := & U_k(\theta,\phi) \left(d_k + d_k^\dagger\right) U_k(\theta,\phi)^\dagger; \\ \sigma_k^{(\theta,\phi)}(y) & := & -iU_k(\theta,\phi) \left(d_k - d_k^\dagger\right) U_k(\theta,\phi)^\dagger; \\ \sigma_k^{(\theta,\phi)}(z) & := & U_k(\theta,\phi) \left(d_k d_k^\dagger - d_k^\dagger d_k\right) U_k(\theta,\phi)^\dagger; \end{array} \tag{42}$$

where

$$U_k(\theta,\phi) := \sin\frac{1}{2}\theta e^{-\frac{1}{2}\phi} d_k + \sin\frac{1}{2}\theta e^{\frac{1}{2}\phi} d_k^\dagger + \cos\frac{1}{2}\theta e^{\frac{1}{2}\phi} d_k d_k^\dagger - \cos\frac{1}{2}\theta e^{-\frac{1}{2}\phi} d_k^\dagger d_k. \tag{43}$$

Intuitively, think of each $U_k(\theta,\phi)$ as rotating eigenstates of spin-direction $\hat{\mathbf{u}}_{(\theta,\phi)}$ to eigenstates of spin-direction $\hat{\mathbf{z}} := \hat{\mathbf{u}}_{(0,0)}$ at spin-site k.

The significant result is now that different choices for (θ,ϕ)—and therefore for $\Omega_{(\theta,\phi)}$—lead to *unitarily inequivalent representations* of the Pauli relations. This can be seen informally by considering that the inner product between any state from $\mathcal{H}_{(\theta,\phi)}$ and any state from $\mathcal{H}_{(\theta',\phi')}$, where $(\theta,\phi) \neq (\theta',\phi')$, involves infinitely many factors of the kind $\langle \theta,\phi | \theta',\phi' \rangle$, each of which is strictly less than one. Therefore, the inner product is zero. This is an instance of representations which are called *disjoint*; we will return to this idea—in later documents ...

Alternatively, note that, for finite spin-sites, the unitary connecting (the analogues of) $\Omega_{(\theta,\phi)}$ and $\Omega_{(0,0)}$ could be implemented by

$$\prod_{k=1}^{n} U_k(\theta,\phi) = \otimes^N \begin{pmatrix} \cos\frac{1}{2}\theta e^{\frac{1}{2}\phi} & \sin\frac{1}{2}\theta e^{-\frac{1}{2}\phi} \\ \sin\frac{1}{2}\theta e^{\frac{1}{2}\phi} & -\cos\frac{1}{2}\theta e^{-\frac{1}{2}\phi} \end{pmatrix} \tag{44}$$

on $\otimes^N \mathbb{C}^2$. But we cannot make sense of the infinite-chain counterpart, i.e. $\prod_{k=-\infty}^{\infty} U_k(\theta,\phi)$, on a separable Hilbert space.

We can see the unitary inequivalence more rigorously by noting that the observables

$$m_{x,n}^{(\theta,\phi)} := \frac{1}{2n+1} \sum_{k=-n}^{n} \sigma_k^{(\theta,\phi)}(x), \quad \text{etc.} \tag{45}$$

defined on $\mathcal{H}_{(\theta,\phi)}$ converge in the weak topology, as $n \to \infty$, to the *global polarization* $\hat{\mathbf{m}}_\infty^{(\theta,\phi)}$, with the expectation value

$$\langle \Omega_{(\theta,\phi)}, \mathbf{m}_\infty^{(\theta,\phi)} \Omega_{(\theta,\phi)} \rangle = \lim_{n\to\infty} \frac{1}{2n+1} \sum_{k=-n}^{n} \hat{\mathbf{u}}_{(\theta,\phi)} = \hat{\mathbf{u}}_{(\theta,\phi)}. \tag{46}$$

Similarly, we can define the global polarization $\hat{\mathbf{m}}_\infty^{(\theta',\phi')}$ in $\mathcal{H}_{(\theta',\phi')}$, where

$$\langle \Omega_{(\theta',\phi')}, \mathbf{m}_\infty^{(\theta',\phi')} \Omega_{(\theta',\phi')} \rangle = \hat{\mathbf{u}}_{(\theta',\phi')}. \tag{47}$$

But $\hat{\mathbf{u}}_{(\theta,\phi)} \neq \hat{\mathbf{u}}_{(\theta',\phi')}$, so these two representations must be unitarily inequivalent.

Some comments:

(i) We can see unitary inequivalence as arising from *"vacuum" polarization.* I.e., the states on which we build each representation differ "infinitely" from each other, and since any two states in the same representation are accessible by a finite number of transformations, any state in one representation will be inaccessible to any state in the other.

(ii) If $N < \infty$, then all states "fit" into a separable Hilbert space, and there is no superselection. But superselection can be approximated for large N by restricting the algebra of quantities to "local" ones.

(iii) How to choose which representation? Answer: sometimes dynamics, sometimes not. E.g. as we have in effect seen above: the ferromagnetic choice $H = \sum_{k=-\infty}^{\infty} (1 - \sigma_k . \sigma_{k+1})$ does not determine a unique vacuum.

(iv) Here, the idea of "particles" (created by our $d^\dagger$ operators) arises as a solution to the problem of defining a Hilbert space of states which is separable, i.e. has a countable basis, for an infinite system (for which we might naturally expect an uncountable number of basis states). That is: here, particles allow us to define finite deviations of the system from a selected "vacuum" state. We say "vacuum" in scare-quotes because (i) we have not invoked a Hamiltonian and (ii) in the spin-chain, the "vacuum" is no more "empty" than any other state. This use of particles also arises in QFT, and is separate from the idea of "particles" associated with finding *normal modes* and their excitations (as discussed in Section 4.1 of Part I).

(v) Unlike in QFT, there is no vacuum entanglement here: i.e. the vacuum state is not entangled between the sites.

(vi) In our later document, *GNS and all that: a rough guide to algebras and states*, we will return to the closing argument above, for unitary inequivalence. We will see it in the context of the facts that (i) the *representations* of a C^*-algebra are given within a Hilbert space, which allows us to define a weak topology; (ii) we can close the set of the C^*-algebra's representatives in this weak topology; and (iii) the new operators so generated (which don't live in the C^*-algebra) have different spectra in different representations; so (iv) they cannot be unitarily equivalent.

(vii) There is also here the general philosophical theme mentioned at the end of Section 2.4.C of Part I: singular limits and emergence.

5 Infinite degrees of freedom 2: the free real boson field

We begin with generalities about symplectic formalisms for classical fields (Section 5.1). Then we give details of the classical Klein-Gordon field (Section 5.2). Then we discuss choices of one-particle structure one can make for this field. In fact there are three natural choices (Section 5.3) which, though unitarily equivalent, differ in the details of their treatments of momentum and, especially, localization (Section 5.4). Then we proceed to the Fock space constructed on a one-particle structure: first in general (Section 5.5), and then for the (now quantum) Klein-Gordon field (Section 5.6). Section 5.7 then discusses, and compares, the field operators defined in terms of the three choices of one-particle structure. Finally, in Section 5.8 we briefly discuss inequivalent representations.

5.1 Classical field theory in general

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It may seem unsatisfactory to begin an introduction to quantum field theory with classical field theory. After all, classical field theory is properly seen as an approximation of the corresponding quantum theory, not the other way around. However, as we shall see, the characterisation of quantum field theory on the approach considered here, which is broadly the approach found in Segal et al., makes essential reference to the classical theory. That is because the quantum theory is characterised in terms of representations of the Weyl algebra; and this algebra is essentially tied to an understanding of the field, whether classical or quantum, as a Hamiltonian dynamical system.

In fact, it will emerge that Weyl algebras not only provide a characterisation of the quantum field, they also provide our best characterisation of *particles*—at least in the case where particles have nonzero mass. In fact, the characterisation of particles in terms of some Weyl algebra extends even to the case where the field is fully regularised on a lattice, where obviously the familiar Lie groups associated with spacetime symmetries do not apply.[1]

The classical field is given by (Γ, Ω), where Γ is a phase space and Ω a symplectic product. Suppose field configurations are given by $q^a : M \to V$, for some measure space (M, μ) and vector space V. So a labels components; and you can often think of M as physical space, as in the first example below.

We then begin with $C_0^\infty(M, V)$ as our space of (smooth, compactly supported) field configurations. Let g_{ab} be an inner product defined on V. Then we can define the inner product on $C_0^\infty(M, V)$ (indicated by round brackets):

$$(q_1, q_2) = \int \mathrm{d}\mu(x)\ g_{mn} q_1^m(x) q_2^n(x) \tag{48}$$

We may then close $C_0^\infty(M, V)$ in the norm induced by this inner product to obtain the real Hilbert space $L^2(M, V, \mu)$.

Field momenta are given by points in the associated space $L^2(M, V^*, \mu)$, and so we may take $\Gamma = L^2(M, V, \mu) \oplus L^2(M, V^*, \mu)$. We will use lowercase Fraktur letters $\mathfrak{z}$ to denote points in Γ; so $\mathfrak{z}$ is shorthand for the pair $(q^a(x), p_b(x)) =: (q^a, p_b)$, where $q^a(x)$ is a classical field configuration and $p_b(x)$ is a classical field momentum. We will usually drop the x and the abstract indices a, b, when they are not needed.

The resulting phase space Γ is also a vector space. The significance of this is that its elements $\mathfrak{z}$ represent not only instantaneous states but also *vectors in* Γ. This will be important for the interpretation of the field quantities. And recall Part I's emphasis on symplectic vector

[1] As we shall see, it is crucial here that there are discrete versions of the Weyl algebra; such versions have no associated Heisenberg algebra. So the Weyl algebras really do provide a general characterisation.

spaces (not merely symplectic manifolds) and linear solution spaces; especially at its Section 3.6.

The symplectic product is given by

$$\Omega(\mathfrak{z}_1, \mathfrak{z}_2) = \Omega((q_1, p^1), (q_2, p^2)) = (q_1, p^2) - (q_2, p^1) \ , \tag{49}$$

where

$$(q_i, p^j) := \int \mathrm{d}\mu(x)\ p^j_n(x) q^n_i(x) \, . \tag{50}$$

(So we use round brackets for both (i) the inner product on pairs of q_is, eq. 48, and (ii) the inner product ('integrated contraction') just defined on q_i, p_j pairs.)

Eq. 50 should be compared with the finite-dimensional symplectic product we defined before: cf. eq.s 7 and 12. Or for details, compare Part I: Section 1.2, especially eq. 1.17; and Section 3.3, especially eq. 3.53.

We can see that, for any $\mathfrak{z} \in \Gamma$, $\Omega(\mathfrak{z}, \ \cdot \ )$ is a real-valued function on Γ, and so it is a classical quantity. Let us call it the *field quantity associated with* $\mathfrak{z}$, and denote it by $\Phi(\mathfrak{z})$.

Choosing $\phi_i(x), \pi^j(x)$ as canonical coordinates on Γ, we can see that

$$\Phi(\mathfrak{z}) := \Omega(\mathfrak{z}, \ \cdot \ ) = \Omega((q,p), \ \cdot \ ) = (q, \pi) - (\phi, p) =: \pi(q) - \phi(p) \tag{51}$$

We have the following Poisson bracket relations between the field quantities $\Phi(\mathfrak{z})$:

$$\{\Phi(\mathfrak{z}_1), \Phi(\mathfrak{z}_2)\} = \{\Omega(\mathfrak{z}_1, \ \cdot \ ), \Omega(\mathfrak{z}_2, \ \cdot \ )\} = \Omega(\mathfrak{z}_1, \mathfrak{z}_2) \tag{52}$$

This is just a concise encapsulation of the familiar Poisson bracket relations:

$$\{\phi(q_1), \phi(q_2)\} = \{\pi(p_1), \pi(p_2)\} = 0 \ ; \qquad \{\phi(p), \pi(q)\} = (q, p) \ . \tag{53}$$

All this recalls the finite-dimensional discussion leading up to eq. 8 above, which is the finite-dimensional analogue of eq. 52 here. (The discussion leading up to eq. 8 summarised Part I, Section 3.3, after eq. 3.54.) There, with a symplectic vector space S as the phase space, $\Omega(z, \cdot)$ for a fixed $z \in S$ was a classical quantity on S. Similarly here in the infinite-dimensional case. For each $\mathfrak{z}$, the field quantity $\Phi(\mathfrak{z})$ has a simple physical interpretation—both as a quantity and as a generator of a family of transformations. Qua quantity, $\Phi(\mathfrak{z})$ is a linear combination of spatially smeared field configuration and momentum quantities. Qua generator, it is the generator of translations in phase space along the vector $\mathfrak{z}$. Particularly salient cases are given (informally) as

$$\begin{aligned} \phi_k(x_0) \ &\equiv \ \phi(\delta_{x_0}\delta_{ik}) \ \equiv \ \Phi(\mathbf{0}, -\delta_{x_0}\delta_{ik}) \ ; & (54) \\ \pi_k(x_0) \ &\equiv \ \pi(\delta_{x_0}\delta_{ik}) \ \equiv \ \Phi(\delta_{x_0}\delta_{ik}, \mathbf{0}) \ ; & (55) \end{aligned}$$

where δ_{x_0} is a Dirac delta distribution centred at $x_0 \in M$ and δ_{ik} is a Kroenecker delta on the indices i, k for some basis for V.

Examples:

- $M = \mathbb{R}^3$ and $V = \mathbb{R}; g = 1$. This describes a real scalar field on 3-space.
- $M = \{\circ\}$ (i.e. the base space is just a one-membered set) and $V = \mathbb{R}^3; g =$ the Euclidean metric. This describes a Euclidean-3-vector-valued "field" on a single point, which is the position of a classical point particle. (We must imagine that physical space has a privileged origin, giving it the structure of a vector space.)

- $M = \{\circ\}$ and $V = \mathbb{R}; g = 1$. This describes the one-dimensional simple harmonic oscillator, and is probably the simplest non-trivial example.

Looking ahead to quantum theory:— Recall that "our main game" has always been to get a formalism in which there is a map from elements z of the classical phase space, first to corresponding classical quantities $\Omega(z, \cdot)$, and then on to quantum quantities i.e. self-adjoint operators $\hat{\Omega}(z, \cdot)$—that is, a map $z \mapsto \hat{\Omega}(z, \cdot)$—with the feature that the corresponding Weyl unitaries

$$W(z) := \exp(i\hat{\Omega}(z, \cdot)) \tag{56}$$

obey the Weyl algebra.

And as we announced in those finite-dimensional discussions just referred to: 'we will later'—i.e. we will in this Section, at last!—use field operators Φ in the sense introduced just above eq. 51, for which (again using hats for quantum operators): $\Phi(Jz) = \hat{\Omega}(z, \cdot)$, or $\Phi(z) = -\hat{\Omega}(Jz, \cdot) = \hat{\Omega}(\cdot, Jz)$. Or in other words, now adopting lowercase Fraktur letters $\mathfrak{z}$ in place of z: we will use field operators Φ, for which $\Phi(J\mathfrak{z}) = \hat{\Omega}(\mathfrak{z}, \cdot)$, or $\Phi(\mathfrak{z}) = -\hat{\Omega}(J\mathfrak{z}, \cdot) = \hat{\Omega}(\cdot, J\mathfrak{z})$.

5.2 Classical Klein-Gordon theory

In classical field theory, the real boson field is represented by a real-valued field on Minkowski spacetime $\phi : \mathbb{R}^4 \to \mathbb{R}$. However, in the Hamiltonian theory—even in relativistic field theory—we envisage the field as a collection of systems parametrized by a *spatial* (not *spatiotemporal*) location $\mathbf{x}$, whose degree of freedom at time t is given by $\phi(\mathbf{x}, t)$. So $\phi(\mathbf{x}, t)$ is to be thought of in analogy with $\mathbf{q}_i(t)$ in classical particle mechanics. As the textbooks often stress: the passage to field theory is characterized by the heuristic that particle labels go over to spatial co-ordinates: $i \mapsto \mathbf{x}$ and position quantities go over to field quantities: $\mathbf{q}_i(t) \mapsto \phi(\mathbf{x}, t)$.

We begin with a configuration space and a Lagrangian density $\mathcal{L}$. The configuration space contains states given pairs of the form $(\phi(\mathbf{x}), \dot{\phi}(\mathbf{x}))$, and the Lagrangian density is

$$\mathcal{L}(\phi(x), \partial_\mu \phi(x)) = \frac{1}{2}\partial^\mu \phi(x)\partial_\mu \phi(x) - \frac{1}{2}m^2\phi(x)^2 \tag{57}$$

(where $\dot{\phi}(\mathbf{x}) \equiv \partial_t \phi(\mathbf{x}, 0)$) To move to the Hamiltonian formalism, we first define, for each $\mathbf{x}$, the conjugate momenta

$$\pi_\phi(\mathbf{x}) := \frac{\partial \mathcal{L}}{\partial \dot{\phi}} = \dot{\phi}(\mathbf{x}). \tag{58}$$

The phase space $S = C_0^\infty(\mathbb{R}^3) \oplus C_0^\infty(\mathbb{R}^3)$ has as elements the pairs $(\phi(\mathbf{x}), \pi_\phi(\mathbf{x}))$. (Here, the *subscript* ϕ on the momentum π is introduced to help us keep track of the two components, configurational and "momentum-al", of the state with configuration ϕ; but of course, π_ϕ is *not* a function of ϕ—it is freely choosable.)

The Hamiltonian is given by

$$H(\phi(\mathbf{x}), \pi_\phi(\mathbf{x})) := \int \mathrm{d}^3\mathbf{x} \, \Big(\pi_\phi(\mathbf{x})\dot{\phi}(\pi_\phi(\mathbf{x})) - \mathcal{L}(\phi(\mathbf{x}), \dot{\phi}(\pi_\phi(\mathbf{x})))\Big) \tag{59}$$

$$= \int \mathrm{d}^3\mathbf{x} \, \frac{1}{2}\left(\pi_\phi(\mathbf{x})^2 + \nabla\phi(\mathbf{x}).\nabla\phi(\mathbf{x}) + m^2\phi(\mathbf{x})^2\right) \tag{60}$$

Note that H will be non-negative for all states. We can integrate the second term in (60) by parts, assuming $\phi(\mathbf{x}) \to 0$ at spatial infinity, to yield

$$H(\phi(\mathbf{x}), \pi_\phi(\mathbf{x})) = \int \mathrm{d}^3\mathbf{x} \, \frac{1}{2}\left(\pi_\phi(\mathbf{x})^2 - \phi(\mathbf{x})\nabla^2\phi(\mathbf{x}) + m^2\phi(\mathbf{x})^2\right) \tag{61}$$

Dynamical solutions are then given by

$$\dot{\phi}(\mathbf{x},t) = \frac{\delta H}{\delta \pi_\phi(\mathbf{x})} = \pi_\phi(\mathbf{x},t); \qquad \dot{\pi}_\phi(\mathbf{x},t) = -\frac{\delta H}{\delta \phi(\mathbf{x})} = \nabla^2\phi(\mathbf{x},t) - m^2\phi(\mathbf{x},t); \tag{62}$$

giving rise to the second-order equation

$$\ddot{\phi}(\mathbf{x},t) = \nabla^2\phi(\mathbf{x},t) - m^2\phi(\mathbf{x},t), \tag{63}$$

which may be expressed as a sum over "on-mass-shell" plane waves:

$$\phi(\mathbf{x},t) = \int \mathrm{d}^3\mathbf{k}\ \frac{1}{\sqrt{2\omega(\mathbf{k})}} \left(a(\mathbf{k})e^{i(\mathbf{k}.\mathbf{x}-\omega(\mathbf{k})t)} + a^*(\mathbf{k})e^{-i(\mathbf{k}.\mathbf{x}-\omega(\mathbf{k})t)} \right) \tag{64}$$

where $\omega(\mathbf{k}) := \mathbf{k}^2 + m^2$. (The reason for the factor $\frac{1}{\sqrt{2\omega(\mathbf{k})}}$ will become clear later.)

The symplectic product on S is given by

$$\Omega(\phi,\psi) \ := \ \int \mathrm{d}^3\mathbf{x}\ \left(\pi_\psi(\mathbf{x})\phi(\mathbf{x}) - \pi_\phi(\mathbf{x})\psi(\mathbf{x})\right). \tag{65}$$

In terms of plane waves, the symplectic form takes the elegant form

$$\Omega(\phi,\psi) = -i\int \mathrm{d}^3\mathbf{k}\ \left(a^*(\mathbf{k})c(\mathbf{k}) - a(\mathbf{k})c^*(\mathbf{k})\right), \tag{66}$$

where $c(\mathbf{k})$ are the momentum amplitudes for ψ. (Here we see convenience of the factor $\frac{1}{\sqrt{2\omega(\mathbf{k})}}$ in (64)).

5.3 The one-particle structure for the Klein-Gordon field: three choices

We begin with frequency-splitting, complex structure and inner product. Then we discuss the three choices for the map K from the classical solution space to the Hilbert space, i.e. the map that intertwines the classical and the quantum dynamics. (Recall the discussion in Section 4.2 of the predecessor document, Part I!) As we mentioned, these choices are unitarily equivalent, but suggestive of different physics—as we will explore in the next Subsection.

TO DO: This Section needs to be augmented with the pedagogic wisdom of Geroch 2005, Sections 1, 3 and 5.

Frequency-splitting

Any state $(\phi(\mathbf{x}), \pi_\phi(\mathbf{x}))$ may be decomposed into positive-frequency and negative-frequency components, according to which

$$\phi(\mathbf{x}) = \phi^{(+)}(\mathbf{x}) + \phi^{(-)}(\mathbf{x}). \tag{67}$$

This is standardly done as follows (see e.g. Wallace (2009, 13)). First, as we have seen, given the Hamiltonian H, any state $(\phi(\mathbf{x}), \pi_\phi(\mathbf{x}))$ defines a unique trajectory $\phi(\mathbf{x},t)$. Taking the frequency-time Fourier transform of this function, we recover a function $\tilde{\phi}(\mathbf{x},\omega)$. We may then define

$$\phi^{(+)}(\mathbf{x}) := \int_0^\infty \mathrm{d}\omega\ \tilde{\phi}(\mathbf{x},\omega); \qquad \phi^{(-)}(\mathbf{x}) := \int_{-\infty}^0 \mathrm{d}\omega\ \tilde{\phi}(\mathbf{x},\omega). \tag{68}$$

Define $A := \sqrt{-\nabla^2 + m^2}$ as an operator on $C_0^\infty(\mathbb{R}^3)$ functions. Then the classical equations of motion may be written

$$\dot{\phi}(\mathbf{x},t) = \frac{\delta H}{\delta \pi_\phi(\mathbf{x})} = \pi_\phi(\mathbf{x},t); \qquad \dot{\pi}_\phi(\mathbf{x},t) = -\frac{\delta H}{\delta \phi(\mathbf{x})} = -A^2\phi(\mathbf{x},t). \tag{69}$$

It may then be checked that

$$\phi^{(+)}(\mathbf{x}) = \frac{1}{2}\left(\phi(\mathbf{x}) + iA^{-1}\pi_\phi(\mathbf{x})\right) = \int \frac{\mathrm{d}^3\mathbf{k}}{\sqrt{2\omega(\mathbf{k})}}\, a(\mathbf{k})e^{i\mathbf{k}.\mathbf{x}}; \tag{70}$$

$$\phi^{(-)}(\mathbf{x}) = \frac{1}{2}\left(\phi(\mathbf{x}) - iA^{-1}\pi_\phi(\mathbf{x})\right) = \int \frac{\mathrm{d}^3\mathbf{k}}{\sqrt{2\omega(\mathbf{k})}}\, a^*(\mathbf{k})e^{-i\mathbf{k}.\mathbf{x}}. \tag{71}$$

Note that $\phi^{(+)}(\mathbf{x})^* = \phi^{(-)}(\mathbf{x})$. The fact that $\phi(\mathbf{x})$ and $\pi_\phi(\mathbf{x})$ are real-valued functions and A is a real operator means that the real (resp. imaginary) parts of $\phi^{(+)}(\mathbf{x})$ and $\phi^{(-)}(\mathbf{x})$ are determined by $\phi(\mathbf{x})$ (resp. $\pi_\phi(\mathbf{x})$).

The complex structure

Define the *complex structure* $J : S \to S$ as follows:

$$J\left(\phi(\mathbf{x}), \pi_\phi(\mathbf{x})\right) := \left(-A^{-1}\pi_\phi(\mathbf{x}), A\phi(\mathbf{x})\right); \tag{72}$$

this is equivalent to

$$J(\phi^{(+)}(\mathbf{x}), \phi^{(-)}(\mathbf{x})) := (i\phi^{(+)}(\mathbf{x}), -i\phi^{(-)}(\mathbf{x})). \tag{73}$$

It may be checked that J satisfies the conditions for a complex structure. We now have a classical "Schrödinger equation":

$$\begin{aligned} J\dot{\phi}(t) &= J(\dot{\phi}(\mathbf{x},t), \dot{\pi}_\phi(\mathbf{x},t)) = J\left(\frac{\delta H}{\delta\pi_\phi(\mathbf{x})}, -\frac{\delta H}{\delta\phi(\mathbf{x})}\right) = J\left(\pi_\phi(\mathbf{x},t), -A^2\phi(\mathbf{x},t)\right) \\ &= (A\phi(\mathbf{x},t), A\pi_\phi(\mathbf{x},t)) = A\phi(t). \end{aligned} \tag{74}$$

This equation diagonalizes, by splitting frequencies, into two "Schrödinger equations":

$$i\dot{\phi}^{(+)}(\mathbf{x},t) = (A\phi^{(+)})(\mathbf{x},t); \qquad -i\dot{\phi}^{(-)}(\mathbf{x},t)) = (A\phi^{(-)})(\mathbf{x},t). \tag{75}$$

The second equation is just the complex conjugate of the first.

The inner product

Recall eq. 13 in Section 1.3 above, and its reference to Part I's discussion of the Kahler condition. Accordingly, our inner product in $C_0^\infty(\mathbb{R}^3)$ is given by

$$\langle\phi,\psi\rangle_S = \frac{1}{2}\Omega(\phi, J\psi) + \frac{1}{2}i\Omega(\phi,\psi) \tag{76}$$

$$= \int \mathrm{d}^3\mathbf{x}\ \frac{1}{2}\left[\phi(\mathbf{x})(A\psi)(\mathbf{x}) + \pi_\phi(\mathbf{x})(A^{-1}\pi_\psi)(\mathbf{x}) + i\left(\pi_\psi(\mathbf{x})\phi(\mathbf{x}) - \pi_\phi(\mathbf{x})\psi(\mathbf{x})\right)\right]. \tag{77}$$

$$= \int \mathrm{d}^3\mathbf{k}\ a^*(\mathbf{k})c(\mathbf{k}) \tag{78}$$

Using the frequency splitting prescription (67) and $\pi_\phi(\mathbf{x}) = -iA(\phi^{(+)}(\mathbf{x}) - \phi^{(-)}(\mathbf{x}))$, and after some laborious calculation, (77) may be written in terms of the positive- and negative-frequency components:

$$\langle\phi,\psi\rangle_S = \int \mathrm{d}^3\mathbf{x}\ \left[\phi^{(-)}(\mathbf{x})(A\psi^{(+)})(\mathbf{x}) + \psi^{(+)}(\mathbf{x})(A\phi^{(-)})(\mathbf{x})\right] \tag{79}$$

$$= 2\int \mathrm{d}^3\mathbf{x}\ \phi^{(-)}(\mathbf{x})(A\psi^{(+)})(\mathbf{x}) \tag{80}$$

$$= \int \mathrm{d}^3\mathbf{x}\ i\phi^{(-)}(\mathbf{x},t)\overleftrightarrow{\partial_t}\psi^{(+)}(\mathbf{x},t), \tag{81}$$

where $f(\mathbf{x},t)\overleftrightarrow{\partial_t}g(\mathbf{x},t) := f(\mathbf{x},t)\partial_t g(\mathbf{x},t) - g(\mathbf{x},t)\partial_t f(\mathbf{x},t)$. Strictly speaking, (81) only makes sense for solutions, since only then do we have any time-dependence; (79) and (80) make sense for instantaneous states, regardless of dynamics.

The map K may be defined in three natural ways, as follows. As we will note at the end of this Section, these three ways are unitarily equivalent. Yet as we shall also see in this Section and the next: they suggest "different physics", especially as regards localization. (More details in e.g. Halvorson (2001), who gives a comparative discussion of the phase-space and Newton-Wigner representations, as they relate to particle localizability).

Phase-space representation
In the phase-space representation we take the map $K_0 : C_0^\infty(\mathbb{R}^3) \oplus C_0^\infty(\mathbb{R}^3) \to \mathcal{H}_0$ to be the embedding map by the identity function. That is: we treat $C_0^\infty(\mathbb{R}^3) \oplus C_0^\infty(\mathbb{R}^3) \ni (\phi(\mathbf{x}), \pi_\phi(\mathbf{x}))$ as itself the pre-Hilbert space ("pre-" because it is not complete in the inner product norm). And we then complete it. We complete the first $C_0^\infty(\mathbb{R}^3)$ in the norm defined by the real inner product

$$\langle \phi(\mathbf{x}), \psi(\mathbf{x})\rangle_1 := \frac{1}{2}\int \mathrm{d}^3\mathbf{x}\ \phi(\mathbf{x})(A\psi)(\mathbf{x}); \tag{82}$$

call the resulting space $\mathcal{L}^+(\mathbb{R}^3)$. We complete the second $C_0^\infty(\mathbb{R}^3)$ in the norm defined by the real inner product

$$\langle \pi_\phi(\mathbf{x}), \pi_\psi(\mathbf{x})\rangle_2 := \frac{1}{2}\int \mathrm{d}^3\mathbf{x}\ \pi_\phi(\mathbf{x})(A^{-1}\pi_\psi)(\mathbf{x}); \tag{83}$$

call the resulting space $\mathcal{L}^-(\mathbb{R}^3)$. Thus the one-particle Hilbert space in this representation is $\mathcal{H}_0 = \mathcal{L}^+(\mathbb{R}^3) \oplus \mathcal{L}^-(\mathbb{R}^3)$. We define the complex inner product in this Hilbert space following (77); i.e. $\langle \phi, \psi\rangle := \langle \phi, \psi\rangle_S = \langle \phi(\mathbf{x}), \psi(\mathbf{x})\rangle_1 + \langle \pi_\phi(\mathbf{x}), \pi_\psi(\mathbf{x})\rangle_2 + \frac{i}{2}\Omega(\phi, \psi)$.

Positive-frequency representation
In the positive-frequency representation, we let the positive frequency component $\phi^{(+)}(\mathbf{x})$ be the quantum representative of the classical wave. So we define the map $K_+ : C_0^\infty(\mathbb{R}^3) \oplus C_0^\infty(\mathbb{R}^3) \to \mathcal{H}_+$ by

$$K_+(\phi(\mathbf{x}), \pi_\phi(\mathbf{x})) := \frac{1}{2}\left(\phi(\mathbf{x}) + iA^{-1}\pi_\phi(\mathbf{x})\right) = \phi^{(+)}(\mathbf{x}). \tag{84}$$

The inner product is defined according to (79):

$$\langle \phi, \psi\rangle := 2\int \mathrm{d}^3\mathbf{x}\ \phi^{(-)}(\mathbf{x})(A\psi^{(+)})(\mathbf{x}). \tag{85}$$

By completing in the norm, we obtain the Hilbert space $\mathcal{H}_+ = L^2(\mathbb{R}^3)$.

Newton-Wigner representation
In the Newton-Wigner representation, which has clear analogies to our treatment above of the simple harmonic oscillator, we define the map $K_{NW} : C_0^\infty(\mathbb{R}^3) \oplus C_0^\infty(\mathbb{R}^3) \to \mathcal{H}_{NW}$ as follows:

$$K_{NW}(\phi(\mathbf{x}), \pi_\phi(\mathbf{x})) := \frac{1}{\sqrt{2}}\left(A^{\frac{1}{2}}\phi(\mathbf{x}) + iA^{-\frac{1}{2}}\pi_\phi(\mathbf{x})\right) =: \phi_{NW}(\mathbf{x}) \equiv \sqrt{2}(A^{\frac{1}{2}}\phi^{(+)})(\mathbf{x}), \tag{86}$$

where $\phi_{NW} : \mathbb{R}^3 \to \mathbb{C}$ is the *complex* wave associated with $(\phi(\mathbf{x}), \pi_\phi(\mathbf{x}))$. This allows us to write the inner product in $C_0^\infty(\mathbb{R}^3) \oplus C_0^\infty(\mathbb{R}^3)$ (77) in the elegant form

$$\langle \phi, \psi\rangle_S = \int \mathrm{d}^3\mathbf{x}\ K_{NW}(\phi)^* K_{NW}(\psi) = \int \mathrm{d}^3\mathbf{x}\ \phi^*_{NW}(\mathbf{x})\psi_{NW}(\mathbf{x}), \tag{87}$$

and so we may define the inner product in $\mathcal{H}_{NW}$ by setting

$$\langle\phi,\psi\rangle := \int \mathrm{d}^3\mathbf{x}\ \phi^*_{NW}(\mathbf{x})\psi_{NW}(\mathbf{x}). \tag{88}$$

By completing in the norm, we find that $\mathcal{H}_{NW} = L^2(\mathbb{R}^3)$. The classical two-component "Schrödinger equation" is mapped under K_{NW} to the single equation

$$i\dot{\phi}_{NW}(\mathbf{x},t) = (A\phi_{NW})(\mathbf{x},t). \tag{89}$$

Given (64) and (86), solutions take the form

$$\phi_{NW}(\mathbf{x},t) = \int \mathrm{d}^3\mathbf{k}\ a(\mathbf{k})e^{i(\mathbf{k}.\mathbf{x}-\omega_{\mathbf{k}}t)}. \tag{90}$$

Happily, all three representations are unitarily equivalent: $K_{NW}\circ K_0^{-1}$, $K\circ K_+^{-1}$, and $K_+\circ K_{NW}^{-1}$ all extend uniquely to unitary operators. This is because all three Hilbert spaces' completions followed the same inner product defined in $C_0^\infty(\mathbb{R}^3)\oplus C_0^\infty(\mathbb{R}^3)$. (But they suggest rival ways to "localize" a state: see Halvorson 2001.)

To sum up: we can specify a one-particle state in any one of three different position representations:

(i) by specifying two real functions $(\phi(\mathbf{x}),\pi_\phi(\mathbf{x}))\in\mathcal{L}^+(\mathbb{R}^3)\oplus\mathcal{L}^-(\mathbb{R}^3)$;
(ii) by specifying a complex function $\phi^{(+)}(\mathbf{x})\in L^2(\mathbb{R}^3)$; or
(iii) by specifying a complex function $\phi_{NW}(\mathbf{x})\in L^2(\mathbb{R}^3)$.

5.4 Eigenstates of momentum—and position?

Recall from our treatment of the simple harmonic oscillator that the map $K : S\to\mathcal{H}$ may obscure which classical states in S lead to which single-particle states in the quantum field. Therefore it is important now to identify familiar eigenstates—particularly of momentum (and position, if possible!)—in the one-particle structure. Only then, when we finally consider the quantum field, will we know which creation and annihilation operators are creating and annihilating which single-particle states. We will now see that in fact, the three different maps K of Section 5.3 exhibit interesting differences from each other.

Phase-space representation:
(Improper) eigenstates of momentum $(\phi_{\mathbf{k}},\pi_{\phi_{\mathbf{k}}})$ are of the form

$$\begin{aligned}\phi_{\mathbf{k}}(\mathbf{x}) &= \frac{1}{\sqrt{2\omega(\mathbf{k})}}\left(e^{i\mathbf{k}.\mathbf{x}}+e^{-i\mathbf{k}.\mathbf{x}}\right) &\equiv \sqrt{\frac{2}{\omega(\mathbf{k})}}\cos(\mathbf{k}.\mathbf{x});\\ \pi_{\phi_{\mathbf{k}}}(\mathbf{x}) &= -i\sqrt{\frac{\omega(\mathbf{k})}{2}}\left(e^{i\mathbf{k}.\mathbf{x}}-e^{-i\mathbf{k}.\mathbf{x}}\right) &\equiv \sqrt{2\omega(\mathbf{k})}\sin(\mathbf{k}.\mathbf{x}).\end{aligned} \tag{91}$$

Positive-frequency representation:
(Improper) eigenstates of momentum $\phi^{(+)}_{\mathbf{k}}$ are of the form

$$\phi^{(+)}_{\mathbf{k}}(\mathbf{x}) = \frac{1}{\sqrt{2\omega(\mathbf{k})}}e^{i\mathbf{k}.\mathbf{x}}\ . \tag{92}$$

Newton-Wigner representation:
(Improper) eigenstates of momentum $\phi^{NW}_{\mathbf{k}}$ are of the form

$$\phi^{NW}_{\mathbf{k}}(\mathbf{x}) = e^{i\mathbf{k}.\mathbf{x}} \; . \tag{93}$$

Each representation represents momentum according to the familiar prescription $(\mathbf{P}\psi)(\mathbf{x}) = -i\nabla\psi(\mathbf{x})$; so we may write $A = \sqrt{\mathbf{P}^2 + m^2}$. And it may be checked that, for each representation,

$$\langle \phi_{\mathbf{k}}, \phi_{\mathbf{l}} \rangle = \frac{1}{2}\left(\sqrt{\frac{\omega(\mathbf{l})}{\omega(\mathbf{k})}} + \sqrt{\frac{\omega(\mathbf{k})}{\omega(\mathbf{l})}} \right) \delta^{(3)}(\mathbf{k}-\mathbf{l}) = \delta^{(3)}(\mathbf{k}-\mathbf{l}); \tag{94}$$

i.e. the eigenstates are orthonormal. Similarly, it may be checked that, for each representation, $\langle \phi, \mathbf{P}\psi \rangle = \langle \mathbf{P}\phi, \psi \rangle$; i.e. $\mathbf{P}$ is self-adjoint. (It is crucial here that $[A, \mathbf{P}] = 0$.)

Note: some authors favour eigenstates $\tilde{\phi}_{\mathbf{k}}$ with a *Lorentz-covariant normalization*, in which $\langle \tilde{\phi}_{\mathbf{k}}, \tilde{\phi}_{\mathbf{l}} \rangle = 2\omega(\mathbf{k})\delta^{(3)}(\mathbf{k}-\mathbf{l})$; see e.g. Duncan (2012, Section 5.2). To obtain this we set, in each representation, $\tilde{\psi} := \sqrt{2}A^{\frac{1}{2}}\psi$ (meaning, for the momentum eigenstates, $\tilde{\phi}_{\mathbf{k}} := \sqrt{2\omega(\mathbf{k})}\phi_{\mathbf{k}}$). The rival choices of normalization may be inter-translated, of course. But we anticipate that, in the field theory, the creation and annihilation operators will satisfy $[a(\phi), a^\dagger(\psi)] = \langle \phi, \psi \rangle$, and it is only when $[a(\phi_{\mathbf{k}}), a^\dagger(\phi_{\mathbf{k}'})] = \delta^{(3)}(\mathbf{k}-\mathbf{k}')$ that these are plausibly construed as ladder operators for the states $\{\phi_{\mathbf{k}}\}$—i.e. in which $a^\dagger(\phi_{\mathbf{k}})$ creates, and $a(\phi_{\mathbf{k}})$ annihilates, a particle in the state $\phi_{\mathbf{k}}$. Therefore *we ought to stick with non-covariant normalization when talking about creating or annihilating particles.*

Position eigenstates?
Surprisingly enough, position is a more complicated matter. To summarize:

(i) the prescription $(\mathbf{Q}\psi)(\mathbf{x}) = \mathbf{x}\psi(\mathbf{x})$ does not lead to the same operator $\mathbf{Q}$ in each representation;

(ii) in some representations this prescription does not even lead to a self-adjoint operator; and

(iii) in the one representation in which we *do* obtain a self-adjoint operator (viz. the Newton-Wigner representation), we run into some troubling features vis a vis relativity.

In fact, the phase-space and positive-frequency representations give rise to the same position operator on the usual prescription. So let us begin by concentrating on the positive-frequency interpretation, because it is simplest. In this representation,

$$\langle \phi, \mathbf{Q}\psi \rangle \;=\; 2\int \mathrm{d}^3\mathbf{x}\; \phi^{(-)}(\mathbf{x}) A\mathbf{x}\psi^{(+)}(\mathbf{x}) \tag{95}$$

$$\;=\; \langle \mathbf{Q}\phi, \psi \rangle + 2\int \mathrm{d}^3\mathbf{x}\; \phi^{(-)}(\mathbf{x})[A, \mathbf{Q}]\psi^{(+)}(\mathbf{x}) \tag{96}$$

By expanding $A = m + \frac{1}{2m}\mathbf{P}^2 + \ldots$, it may be checked that $[A, \mathbf{Q}] = -iA^{-1}\mathbf{P}$. So

$$\langle \phi, \mathbf{Q}\psi \rangle - \langle \mathbf{Q}\phi, \psi \rangle = -\langle \phi, iA^{-2}\mathbf{P}\psi \rangle, \tag{97}$$

which in general is non-zero, so $\mathbf{Q}$ is not self-adjoint. Accordingly, it may be checked that the "eigenstates" $\xi^{(+)}_{\mathbf{x}_0} := \delta^{(3)}(\mathbf{x}-\mathbf{x}_0)$ are not orthogonal:

$$\langle \xi^{(+)}_{\mathbf{x}}, \xi^{(+)}_{\mathbf{y}} \rangle = 2\int \mathrm{d}^3\mathbf{z}\; \delta^{(3)}(\mathbf{z}-\mathbf{x}) A \delta^{(3)}(\mathbf{z}-\mathbf{y}) = 2A\delta^{(3)}(\mathbf{x}-\mathbf{y}) = 2\int \mathrm{d}^3\mathbf{k}\; \omega(\mathbf{k}) e^{i\mathbf{k}.(\mathbf{x}-\mathbf{y})}. \tag{98}$$

However, we may contrive a self-adjoint operator by defining

$$\mathbf{Q}_{NW} := \mathbf{Q} + \frac{i}{2}A^{-2}\mathbf{P}. \tag{99}$$

This ensures that $\langle \phi, \mathbf{Q}_{NW}\psi \rangle = \langle \mathbf{Q}_{NW}\phi, \psi \rangle$, since $[A, \mathbf{P}] = 0$ and A and $\mathbf{P}$ are self-adjoint. It may also be checked that $[A^{\frac{1}{2}}, \mathbf{Q}] = -\frac{i}{2}A^{-\frac{3}{2}}\mathbf{P}$. Using this, we find that

$$\begin{aligned} A^{-\frac{1}{2}}\mathbf{Q}A^{\frac{1}{2}} &= \mathbf{Q} + A^{-\frac{1}{2}}[\mathbf{Q}, A^{\frac{1}{2}}] \\ &= \mathbf{Q} + \frac{i}{2}A^{-2}\mathbf{P} \\ &= \mathbf{Q}_{NW}. \end{aligned} \tag{100}$$

$\mathbf{Q}_{NW}$ is called the *Newton-Wigner position operator* for the very good reason that, in the Newton-Wigner representation,

$$(\mathbf{Q}_{NW}\psi_{NW})(\mathbf{x}) = \mathbf{x}\psi_{NW}(\mathbf{x}), \tag{101}$$

as per the usual prescription.

Accordingly, the (improper) eigenstates of $\mathbf{Q}_{NW}$ are Dirac delta functions *in the Newton-Wigner representation.* In the phase-space representation, they are given by $(\phi_{\mathbf{x}_0}, \pi_{\mathbf{x}_0})$, where $\pi_{\mathbf{x}_0} = \mathbf{0}$ and

$$\phi_{\mathbf{x}_0}(\mathbf{x}) = \int \mathrm{d}^3\mathbf{k}\ \frac{1}{\sqrt{2\omega(\mathbf{k})}}\left(e^{i\mathbf{k}.(\mathbf{x}-\mathbf{x}_0)} + e^{-i\mathbf{k}.(\mathbf{x}-\mathbf{x}_0)}\right) = \int \mathrm{d}^3\mathbf{k}\ \sqrt{\frac{2}{\omega(\mathbf{k})}}\cos\mathbf{k}.(\mathbf{x}-\mathbf{x}_0). \tag{102}$$

In the positive-frequency representation, we have $\phi^{(+)}_{\mathbf{x}_0}(\mathbf{x}) = \int \mathrm{d}^3\mathbf{k}\ \frac{1}{\sqrt{2\omega(\mathbf{k})}}e^{i\mathbf{k}.(\mathbf{x}-\mathbf{x}_0)}$.

Despite its obvious attractions, the Newton-Wigner standard of localization raises a handful of worries with regard to its appropriateness for a relativistic theory.

(i) The Newton-Wigner position eigenstates have infinite tails in the other two representations.

(ii) Even in the Newton-Wigner representation, states localized at one time become unlocalized arbitrarily soon, due to A's being an *anti-local* operator. (An anti-local operator B is one such that, for any $\mathbf{0} \neq \phi_{NW}(\mathbf{x}) \in L^2(\mathbb{R}^3)$ and any open region $O \subset \mathbb{R}^3$, if $\mathrm{supp}(\phi_{NW}(\mathbf{x})) \cap O = \varnothing$, then $\mathrm{supp}(B\phi_{NW}(\mathbf{x})) \cap O \neq \varnothing$.) Paradoxically, the Newton-Wigner velocity operator nevertheless satisfies

$$\dot{\mathbf{Q}}_{NW} = -i[\mathbf{Q}_{NW}, A] = i[A, \mathbf{Q}] = A^{-1}\mathbf{P}, \tag{103}$$

whose spectrum is the interior of the unit ball (the velocity never reaches or exceeds 1).

(iii) Relatedly, Newton-Wigner localization is not Lorentz-covariant. Specifically, any state which is localized at some time in the Newton-Wigner position associated with *one* inertial frame is *un*localized at *all* times in the Newton-Wigner position associated with *any* other inertial frame. This gives rise to the failure of projectors associated with spatial regions which are spacelike-separated but nonsimultaneous to commute.

It is worth emphasizing that it was never guaranteed that a position operator *would* be found on the one-particle structure, and it is no paradox if there isn't one. We are seeking a representation of the Weyl algebra over the space of classical field configurations $C_0^\infty(\mathbb{R}^3) \oplus C_0^\infty(\mathbb{R}^3)$, *not* a representation of the Weyl algebra over the classical particle phase space $\mathbb{R}^6$.

So much by way of looking at various one-particle structure. We turn (at last!) to quantum field theory, i.e. variable particle-number, as formulated in terms of Fock space ...

5.5 The free bosonic field on any one-particle structure: the general idea recalled

In this Section, we present the idea of Fock space in a mathematical way. Similar presentations are in e.g. Baez et al.(1992, Sections 1.8, 1.9), Araki (1993, Section 3.5), Folland (2008, Section 4.5), and De Faria and De Melo. More physics-oriented presentations include e.g.: Schweber, *Introduction to Relativistic Quantum Field Theory* (1961, Chapters 6 and 7), Loudon, *The Quantum Theory of Light* (1973: Chapters 6 and 7), Itzykson and Zuber, *Quantum Field Theory* (1987, Section 3.1), Coleman *Lectures on Quantum Field Theory* (2019, Chapters 2,3,4). (And cf. Section 4, especially Section 4.4 of the predecessor document, Part I.)

Once we have our one-particle system $(\mathcal{H}, \langle\cdot,\cdot,\rangle, U(t))$, we may define the *free boson field over* it. *This quantum theory will provide a representation of our Weyl algebra.* Besides, the following prescription is unique, up to unitary equivalence; see Baez *et al* 1992, pp. 49-56, Theorem 1.10.

The free boson field over $\mathcal{H}$ is the system $(\mathfrak{F}_+(\mathcal{H}), W, \Gamma, \nu)$ where

$$\mathfrak{F}_+(\mathcal{H}) := \bigoplus_{n=0}^{\infty} \mathcal{S}_n\left(\otimes^n \mathcal{H}\right) \tag{104}$$

is the Hilbert space of all symmetric tensors on $\mathcal{H}$, and for any linear operator $Q \in \mathcal{B}(\mathcal{H})$,

$$\Gamma(Q) := 1 \oplus Q \oplus (Q \otimes Q) \oplus (Q \otimes Q \otimes Q) \oplus \ldots|_{\mathfrak{F}_+(\mathcal{H})} . \tag{105}$$

We assume a strongly continuous one-parameter family $U(t)$ of unitaries on $\mathcal{H}$, which is generated by some self-adjoint operator A. The corresponding family $\Gamma(U(t))$, is generated by a self-adjoint operator which we call $\mathrm{d}\Gamma(A)$. It satisfies

$$\Gamma(U(t)) = \Gamma(e^{itA}) = e^{it\mathrm{d}\Gamma(A)} \tag{106}$$

and

$$\mathrm{d}\Gamma(A) := 0 \oplus A \oplus (A \otimes \mathbb{1} + \mathbb{1} \otimes A) \oplus \ldots|_{\mathfrak{F}_+(\mathcal{H})} . \tag{107}$$

Finally, the *vacuum state* ν is defined by

$$\nu = 1 \oplus \mathbf{0} \oplus \mathbf{0} \oplus \ldots \tag{108}$$

Note that it then satisfies

$$\Gamma(U(t))\nu = \nu. \tag{109}$$

Now we describe how the free bosonic field $(\mathfrak{F}_+(\mathcal{H}), W, \Gamma, \nu)$ provides a representation for the Weyl algebra.

We need to define, for every $\xi \in \mathcal{H}$, creation and annihilation operators $a^\dagger(\xi), a(\xi)$; $\mathfrak{F}_+(\mathcal{H})$ is the closed linear span of arbitrary combinations of these acting on ν. To this end we define the operators $a^\dagger_{(N)}(\xi) : \otimes^{N-1}\mathcal{H} \to \otimes^N \mathcal{H}$ and $a_{(N)}(\xi) : \otimes^N \mathcal{H} \to \otimes^{N-1}\mathcal{H}$ for all $N \in \mathbb{N}$:

$$\begin{array}{rcl} a^\dagger_{(N)}(\xi)\,(\psi_1 \otimes \ldots \otimes \psi_{N-1}) & := & \xi \otimes \psi_1 \otimes \ldots \otimes \psi_{N-1} \\ a_{(N)}(\xi)\,(\psi_1 \otimes \psi_2 \otimes \ldots \otimes \psi_N) & := & \langle \xi, \psi_1 \rangle\ \psi_2 \otimes \ldots \otimes \psi_N \end{array} \tag{110}$$

where $\chi_k(j) = \delta_{jk}$. Now we may define $a^\dagger(\xi), a(\xi) : \mathfrak{F}_+(\mathcal{H}) \to \mathfrak{F}_+(\mathcal{H})$ by

$$\begin{array}{rcccccccc} a^\dagger(\xi) & := & a^\dagger_{(1)}(\xi) & \oplus & \sqrt{2}\mathcal{S}_2 a^\dagger_{(2)}(\xi) & \oplus & \sqrt{3}\mathcal{S}_3 a^\dagger_{(3)}(\xi) & \oplus & \ldots \\ a(\xi) & := & 0 & \oplus & a_{(1)}(\xi) & \oplus & \sqrt{2} a_{(2)}(\xi) & \oplus & \sqrt{3} a_{(3)}(\xi) \oplus \ldots \end{array} \tag{111}$$

It may be checked that

$$[a(\xi_1), a(\xi_2)] = [a^\dagger(\xi_1), a^\dagger(\xi_2)] = 0; \qquad [a(\xi_1), a^\dagger(\xi_2)] = \langle \xi_1, \xi_2 \rangle; \tag{112}$$

this will be crucial for representing the Weyl algebra. We also have, for any projector P on $\mathcal{H}$,

$$\mathrm{d}\Gamma(P) = \sum_i \mathrm{d}\Gamma(\Pi(\xi_i)) = \sum_i a^\dagger(\xi_i) a(\xi_i), \tag{113}$$

where the ξ_i are an orthonormal basis for $\mathrm{ran}(P)$ and $\Pi(\xi_i)$ projects onto the ray spanned by ξ_i.

We now define the (unbounded) field operators for all $z \in S$:

$$\Phi(z) := a(K(z)) + a^\dagger(K(z)), \tag{114}$$

where $K : S \to \mathcal{H}$ is our map from the classical phase space to the single-particle Hilbert space. It follows from (112) that, for all $z_1, z_2 \in S$ in a dense domain,

$$\begin{aligned}
[\Phi(z_1), \Phi(z_2)] &= [a(K(z_1)), a^\dagger(K(z_2))] + [a^\dagger(K(z_1)), a(K(z_2))] \\
&= -2i\Im m\langle K(z_1), K(z_2)\rangle = -i\Omega(z_1, z_2),
\end{aligned} \tag{115}$$

Equation (115) is none other than our Weyl relations in infinitesimal form. The representation $W : S \to \mathfrak{B}\left[\mathfrak{F}_+(\mathcal{H})\right]$ of the Weyl algebra is then provided by

$$W(z) := e^{i\Phi(Jz)}. \tag{116}$$

The "particle picture"
For any projector P on $\mathcal{H}$, the operator $\mathrm{d}\Gamma(P)$ is the particle number operator associated with P. The total particle number operator is $N := \mathrm{d}\Gamma(\mathbb{1})$. Eigenstates of N are states of the field with definite particle number.

The "real wave picture"
For each $z \in S$, the field operator $\Phi(Jz)$ is the unique self-adjoint operator which generates the strongly continuous one-parameter family of unitaries $W(tz)$, where $t \in \mathbb{R}$. Eigenstates of $\Phi(Jz)$ do not, strictly speaking, exist, but $\Phi(Jz)$ admits of a spectral decomposition, in analogy with $\mathbf{Q}$ and $\mathbf{P}$ in elementary nonrelativistic quantum mechanics.

The "complex wave picture"
Here the relevant operators are the creation and annihilation operators, for any $z \in S$:

$$a^\dagger(K(z)) = \frac{1}{2}\left(\Phi(z) - i\Phi(Jz)\right); \qquad a(K(z)) = \frac{1}{2}\left(\Phi(z) + i\Phi(Jz)\right) \tag{117}$$

The relevant "eigenstates" are of $a(K(z))$ (a misleading term, since $a(K(z))$ is not a normal operator). These are coherent states.

Note that there is a natural sense in which the field operator is a function over the *classical* phase space S, while the creation and annihilation operators are functions over the *quantum* one-particle Hilbert space $\mathcal{H}$.

5.6 The free Klein-Gordon field

By picking one of our three one-particle structures $(\mathcal{H}, \langle\cdot,\cdot\rangle, U(t))$, from Section 5.3, we may define the free bosonic Klein-Gordon field, which will provide a representation of the Weyl algebra over $S = C_0^\infty(\mathbb{R}^3) \oplus C_0^\infty(\mathbb{R}^3)$. We emphasize that any two choices lead to equivalent theories, since as mentioned at the start of Section 5.5: its prescription for building Fock space is unique, up to unitary equivalence; see Baez *et al* 1992, pp. 49-56, Theorem 1.10.

The free boson field over $\mathcal{H}$ is the system $(\mathfrak{F}_+(\mathcal{H}), W, \Gamma, \nu)$ where

$$\mathfrak{F}_+(\mathcal{H}) := \bigoplus_{n=0}^{\infty} \mathcal{S}_n \left(\otimes^n \mathcal{H}\right). \tag{118}$$

Γ is defined, for any linear operator $Q \in \mathcal{B}(\mathcal{H})$, by

$$\Gamma(Q) := 1 \oplus Q \oplus (Q \otimes Q) \oplus (Q \otimes Q \otimes Q) \oplus \ldots|_{\mathfrak{F}_+(\mathcal{H})}. \tag{119}$$

Dynamical evolution is governed by the strongly continuous one-parameter family of unitaries $\Gamma(U(t))$, which is generated by the self-adjoint operator

$$\mathrm{d}\Gamma(A) := 0 \oplus A \oplus (A \otimes \mathbb{1} + \mathbb{1} \otimes A) \oplus \ldots|_{\mathfrak{F}_+(\mathcal{H})}. \tag{120}$$

The *vacuum state* ν is defined by

$$\nu = 1 \oplus \mathbf{0} \oplus \mathbf{0} \oplus \ldots \tag{121}$$

so that $\Gamma(U(t))\nu = \nu$.

We define the creation and annihilation operators $a^\dagger, a : \mathcal{H} \to \mathfrak{B}(\mathfrak{F}_+(\mathcal{H}))$ in the usual way (see Section 5.5), and we have, for any $\xi_1, \xi_2 \in \mathcal{H}$,

$$[a(\xi_1), a(\xi_2)] = [a^\dagger(\xi_1), a^\dagger(\xi_2)] = 0; \qquad [a(\xi_1), a^\dagger(\xi_2)] = \langle \xi_1, \xi_2 \rangle. \tag{122}$$

A very important property of Γ is that

$$\Gamma(Q) a^\dagger(\xi) \Gamma(Q)^{-1} = a^\dagger(Q\xi); \qquad \Gamma(Q) a(\xi) \Gamma(Q)^{-1} = a(Q\xi) \tag{123}$$

for *any* invertible operator Q and state ξ in the one-particle structure $\mathcal{H}$. We are interested in the creation and annihilation of momentum eigenstates, for which

$$a^\dagger(\mathbf{k}) := a_S^\dagger\left(\sqrt{\frac{2}{\omega(\mathbf{k})}}\cos(\mathbf{k}.\mathbf{x}), \sqrt{2\omega(\mathbf{k})}\sin(\mathbf{k}.\mathbf{x})\right) \equiv a_{(+)}^\dagger\left(\frac{e^{i\mathbf{k}.\mathbf{x}}}{\sqrt{2\omega(\mathbf{k})}}\right) \equiv a_{NW}^\dagger\left(e^{i\mathbf{k}.\mathbf{x}}\right), \tag{124}$$

where the subscripts 'S', '$(+)$' and 'NW' correspond to the phase-space, positive-frequency and Newton-Wigner representations, respectively. It may be checked that

$$[a(\mathbf{k}), a(\mathbf{l})] = [a^\dagger(\mathbf{k}), a^\dagger(\mathbf{l})] = 0; \qquad [a(\mathbf{k}), a^\dagger(\mathbf{l})] = \delta^{(3)}(\mathbf{k} - \mathbf{l}). \tag{125}$$

We now define the (unbounded) field operators for all $z \in S$:

$$\Phi(z) := a_K(K(z)) + a_K^\dagger(K(z)), \tag{126}$$

where $K : S \to \mathcal{H}$ defines our representation; i.e. the map from the classical phase space to the single-particle Hilbert space. Note that, since Φ is a function over S, it is representation-independent. We can expand any field operator in terms of momentum ladder operators in a way that is independent of representation. Going via the positive-frequency representation for convenience, any state $\phi^{(+)}(\mathbf{x})$ is mapped to the field operator

$$\Phi\left(K_+^{-1}\left(\phi^{(+)}(\mathbf{x})\right)\right) = a_{(+)}\left(\phi^{(+)}(\mathbf{x})\right) + a^\dagger_{(+)}\left(\phi^{(+)}(\mathbf{x})\right). \tag{127}$$

We may express $\phi^{(+)}(\mathbf{x})$ in terms of plane waves:

$$\phi^{(+)}(\mathbf{x}) = \int \mathrm{d}^3\mathbf{k}\ \frac{c(\mathbf{k})e^{i\mathbf{k}.\mathbf{x}}}{\sqrt{2\omega(\mathbf{k})}}, \tag{128}$$

and use the complex linearity (resp., complex anti-linearity) of $a^\dagger$ (resp., a) to obtain

$$\Phi\left(K_+^{-1}\left(\phi^{(+)}(\mathbf{x})\right)\right) = \int \mathrm{d}^3\mathbf{k}\ \left[c^*(\mathbf{k})a_{(+)}\left(\frac{e^{i\mathbf{k}.\mathbf{x}}}{\sqrt{2\omega(\mathbf{k})}}\right) + c(\mathbf{k})a^\dagger_{(+)}\left(\frac{e^{i\mathbf{k}.\mathbf{x}}}{\sqrt{2\omega(\mathbf{k})}}\right)\right] \tag{129}$$

$$= \int \mathrm{d}^3\mathbf{k}\ \left[c^*(\mathbf{k})a(\mathbf{k}) + c(\mathbf{k})a^\dagger(\mathbf{k})\right]. \tag{130}$$

This holds also for the other two representations. In particular, we may interpret

$$\Phi(\mathbf{k}) := \Phi\left(K^{-1}(\phi_\mathbf{k})\right) = a(\mathbf{k}) + a^\dagger(\mathbf{k}) \tag{131}$$

(where $\phi_\mathbf{k}$ is the improper momentum eigenstate associated with the eigenvalue $\mathbf{k}$) as the quantum observable corresponding to the amplitude of the $\mathbf{k}$ momentum mode. It may be checked that $[\Phi(\mathbf{k}), \Phi(\mathbf{l})] = [a(\mathbf{k}), a^\dagger(\mathbf{l})] + [a^\dagger(\mathbf{k}), a(\mathbf{l})] = 0$.

Finally, the representation $W : S \to \mathfrak{B}\left[\mathfrak{F}_+(\mathcal{H})\right]$ of the Weyl algebra on S is provided, as usual, by

$$W(z) := e^{i\Phi(Jz)}. \tag{132}$$

Given the definitions above, we also have that (see Baez *at al* 1992, pp. 34-35)

$$\langle \nu, W(z)\nu\rangle = e^{-\frac{1}{2}\|z\|^2}, \tag{133}$$

where $\|z\|^2 := \langle z, z\rangle_S$ is the squared norm of z in the one-particle structure. We use the fact that the $\Phi(z)$ are self-adjoint and that, for any operators A and B which commute with their commutator $[A, B]$, $e^{A+B} = e^{-\frac{1}{2}[A,B]}e^A e^B$. This result is extremely helpful, since for each $z \in S$, $\langle \nu, W(tz)\nu\rangle = \langle \nu, e^{it\Phi(z)}\nu\rangle$ (with $t \in \mathbb{R}$), known in the theory of random variables as the *characteristic function* of the random variable $\Phi(z)$, completely determines the probability distribution of $\Phi(z)$ in the vacuum state ν (it is its inverse Fourier transform).

The "particle picture"

For any projector Π on $\mathcal{H}$, the operator $\mathrm{d}\Gamma(\Pi)$ is the particle number operator associated with Π. The total particle number operator is $N := \mathrm{d}\Gamma(\mathbb{1})$. Eigenstates of N are states of the field with definite particle number. The Hamiltonian for the field is

$$H := \mathrm{d}\Gamma(A) = \mathrm{d}\Gamma\left(\sqrt{\mathbf{P}^2 + m^2}\right) = \mathrm{d}\Gamma\left(\int \mathrm{d}^3\mathbf{k}\ \omega(\mathbf{k})\Pi(\mathbf{k})\right), \tag{134}$$

where $\Pi(\mathbf{k})$ is the (improper) projector onto the (improper) momentum eigenstate $\phi_\mathbf{k}$. Using the fact that $\mathrm{d}\Gamma$ is linear, we obtain the familiar result

$$H = \int \mathrm{d}^3\mathbf{k}\ \omega(\mathbf{k})\mathrm{d}\Gamma\left(\Pi(\mathbf{k})\right) = \int \mathrm{d}^3\mathbf{k}\ \omega(\mathbf{k})a^\dagger(\mathbf{k})a(\mathbf{k}). \tag{135}$$

The "real wave picture"
For each $z \in S$, the field operator $\Phi(Jz)$ is the unique self-adjoint operator which generates the strongly continuous one-parameter family of unitaries $W(tz)$, where $t \in \mathbb{R}$. Eigenstates of $\Phi(Jz)$ do not, strictly speaking, exist, but $\Phi(Jz)$ admits of a spectral decomposition, in analogy with $\mathbf{Q}$ and $\mathbf{P}$ in elementary nonrelativistic quantum mechanics. In the next section we will discuss "local" field operators (i.e. field operators associated with spatial or spacetime points) in detail.

An important theorem applies here (see Baez, Segal & Zhou 1992, Corollary 1.10.3, p. 57):

Theorem 5.1 ("Wave-particle duality")**.** *Let $\mathcal{H}_{\mathbb{R}}$ be the real subspace of the one-particle Hilbert space $\mathcal{H}$. The bosonic Fock space $\mathfrak{F}_+(\mathcal{H})$ is unitarily equivalent to the space $L^2(M)$, where M is the tensor product of* $\dim(\mathcal{H}_{\mathbb{R}})$ *copies of* $(\mathbb{R}, g_c)$*, where $dg_c := \frac{1}{\sqrt{2\pi c}} e^{-\frac{x^2}{2c}} dx$ (known as the isonormal distribution).*

In the case where $\mathcal{H} = L^2(\mathbb{R}^3)$, the space of classical waves M is $L^2(\mathbb{R}^3, \mathbb{R}, g_c)$; i.e. real-valued functions over $\mathbb{R}^3$.

5.7 What are the "local" field operators?

In standard presentations, one finds the "local" field operator $\Phi(\mathbf{x})$, which one is encouraged to interpret as the quantum observable associated with the amplitude of the field at $\mathbf{x}$. We are now in a position to identify these operators.

Recall that for the simple harmonic oscillator, $Q = \Phi(J(0, -1)) = \Phi(\frac{1}{m\omega}, 0)$. For a system of coupled harmonic oscillators, this generalizes to $Q_i = \Phi(J(\mathbf{0}, -\delta_{ik})) = \Phi(\tilde{A}^{-1}\delta_{ik}, \mathbf{0})$, where $\tilde{A} := \sqrt{-\partial_+\partial_- + m^2}$ is the discrete analogue of A. So in the field theory (the continuum limit of the series of coupled oscillators), we should expect that (e.g. in the positive-frequency representation)

$$\begin{aligned}
\Phi(\mathbf{x}_0) &= \Phi(J(\mathbf{0}, -\delta^{(3)}(\mathbf{x} - \mathbf{x}_0)) = \Phi(A^{-1}\delta^{(3)}(\mathbf{x} - \mathbf{x}_0), \mathbf{0}) && (136)\\
&= a_{(+)}\left[\frac{1}{2}A^{-1}\delta^{(3)}(\mathbf{x} - \mathbf{x}_0)\right] + a^\dagger_{(+)}\left[\frac{1}{2}A^{-1}\delta^{(3)}(\mathbf{x} - \mathbf{x}_0)\right] && (137)\\
&= a_{(+)}\left[\int \frac{\mathrm{d}^3\mathbf{k}}{2\omega(\mathbf{k})} e^{i\mathbf{k}.(\mathbf{x}-\mathbf{x}_0)}\right] + a^\dagger_{(+)}\left[\int \frac{\mathrm{d}^3\mathbf{k}}{2\omega(\mathbf{k})} e^{i\mathbf{k}.(\mathbf{x}-\mathbf{x}_0)}\right] && (138)\\
&= a_{(+)}\left[\psi^{(+)}_{(\mathbf{x}_0,t_0)}(\mathbf{x}, t_0)\right] + a^\dagger_{(+)}\left[\psi^{(+)}_{(\mathbf{x}_0,t_0)}(\mathbf{x}, t_0)\right], && (139)
\end{aligned}$$

where

$$\begin{aligned}
\psi^{(+)}_{(\mathbf{x}_0,t_0)}(\mathbf{x}, t) &:= \int \frac{\mathrm{d}^3\mathbf{k}}{2\omega(\mathbf{k})} e^{-i[\omega(\mathbf{k})(t-t_0) - \mathbf{k}.(\mathbf{x}-\mathbf{x}_0)]} && (140)\\
&= \int \mathrm{d}^4k \; \delta(k_0^2 - \omega(\mathbf{k})^2)\Theta(k_0) e^{-ik\cdot(x-x_0)} && (141)\\
&= \Pi^+(m)\delta^{(4)}(x - x_0) \;=\; i\Delta^{(+)}(x - x_0), && (142)
\end{aligned}$$

using $\int \mathrm{d}k_0 \; \delta(k_0^2 - \alpha^2)\Theta(k_0) = \frac{1}{2\alpha}$, and where $\Pi^+(m)$ is the projector onto the positive-frequency mass shell, defined by $k^2 \equiv k_0^2 - \mathbf{k}^2 = m^2$ and $k_0 > 0$, and $\Delta^{(+)}(x)$ is the *positive-frequency Pauli-Jordan function*, which has spacelike tails. (For a full discussion of this and related functions, see Greiner & Reinhardt (1996, Section 4.6).) Using (138) and the fact that eigenstates of momentum in the positive-frequency representation are $\frac{1}{\sqrt{2\omega(\mathbf{k})}}e^{i\mathbf{k}.\mathbf{x}}$, we see that

$$\Phi(\mathbf{x}_0) = \int \frac{\mathrm{d}^3\mathbf{k}}{\sqrt{2\omega(\mathbf{k})}} \left[a(\mathbf{k})e^{i\mathbf{k}.\mathbf{x}_0} + a^\dagger(\mathbf{k})e^{-i\mathbf{k}.\mathbf{x}_0}\right], \tag{143}$$

which is the expression for the local field operators found in textbooks.

What is potentially confusing about this result is that, although (143) gives the right expression for the local field operators, its positive- and negative-frequency parts are *not* ladder operators associated with a localized state in the one-particle structure. Let us investigate this further in each of the three representations (this time we will take the positive-frequency representation first).

Positive-frequency representation

Given (139) and (142), the ladder operators $a_{(+)}(\psi^{(+)}_{x_0}), a^\dagger_{(+)}(\psi^{(+)}_{x_0})$ associated with the local field operator $\Phi(x_0)$ create or annihilate a single particle in the state $\psi^{(+)}_{x_0}(x) = i\Delta^{(+)}(x - x_0)$. This function is a solution to the positive-frequency representation's Schrödinger equation:

$$i\partial_t\Delta^{(+)}(x - x_0) = A\Delta^{(+)}(x - x_0). \tag{144}$$

Phase-space representation

In the phase-space representation, this state is given by $(\psi_{(\mathbf{x}_0,t_0)}(\mathbf{x}, t), \pi_{(\mathbf{x}_0,t_0)}(\mathbf{x}, t))$, where

$$\begin{aligned}
\psi_{(\mathbf{x}_0,t_0)}(\mathbf{x}, t) &:= \int \frac{\mathrm{d}^3\mathbf{k}}{2\omega(\mathbf{k})} \left(e^{-i[\omega(\mathbf{k})(t-t_0)-\mathbf{k}.(\mathbf{x}-\mathbf{x}_0)]} + e^{i[\omega(\mathbf{k})(t-t_0)-\mathbf{k}.(\mathbf{x}-\mathbf{x}_0)]}\right) && (145)\\
&= \int \mathrm{d}^4k\ \delta(k_0^2 - \omega(\mathbf{k})^2)e^{-ik\cdot(x-x_0)} && (146)\\
&= \Pi(m)\delta^{(4)}(x - x_0)\ =\ i\Delta_1(x - x_0) && (147)
\end{aligned}$$

and

$$\begin{aligned}
\pi_{(\mathbf{x}_0,t_0)}(\mathbf{x}, t) &:= -i\int \mathrm{d}^3\mathbf{k}\ \frac{1}{2} \left(e^{-i[\omega(\mathbf{k})(t-t_0)-\mathbf{k}.(\mathbf{x}-\mathbf{x}_0)]} - e^{i[\omega(\mathbf{k})(t-t_0)-\mathbf{k}.(\mathbf{x}-\mathbf{x}_0)]}\right) && (148)\\
&= -i\int \mathrm{d}^4k\ A\delta(k_0^2 - \omega(\mathbf{k})^2)\Theta(k_0)e^{-ik\cdot(x-x_0)} && (149)\\
&= -iA\left(\Pi^+(m)\delta^{(4)}(x - x_0) - \Pi^-(m)\delta^{(4)}(x - x_0)\right) && (150)\\
&= \partial_t\Pi(m)\delta^{(4)}(x - x_0)\ =\ A\Delta(x - x_0), && (151)
\end{aligned}$$

where $\Pi(m) \equiv \Pi^+(m)+\Pi^-(m)$ projects onto the full $k^2 = m^2$ mass-shell, $\Pi^-(m)$ projects onto the negative-frequency mass-shell, the real-valued function $\Delta(x) \equiv \Delta^{(+)}(x) + \Delta^{(-)}(x)$ (where $\Delta^{(-)}(x) := \Delta^{(+)}(x)^*$) is the *Pauli-Jordan function*, and the pure-imaginary-valued function $\Delta_1(x) \equiv \Delta^{(+)}(x) - \Delta^{(-)}(x)$ is the *Pauli-Jordan anticommutator* (see Greiner & Reinhardt (1996, Section 4.6)). The functions $\Delta(x)$ and $\Delta_1(x)$ are related by

$$i\partial_t\Delta(x) = A\Delta_1(x); \qquad i\partial_t\Delta_1(x) = A\Delta(x); \tag{152}$$

and are connected by the complex structure J according to

$$\begin{aligned}
J\left(\Delta(x), -iA\Delta_1(x)\right) &= \left(i\Delta_1(x), A\Delta(x)\right); && (153)\\
J\left(i\Delta_1(x), A\Delta(x)\right) &= \left(-\Delta(x), iA\Delta_1(x)\right). && (154)
\end{aligned}$$

$\Delta_1(x)$, like $\Delta^{(+)}(x)$, has spacelike tails, but we can use the fact that $\Delta(-x) = -\Delta(x)$ and $\Delta(x)$ is Lorentz-invariant to show that $\Delta(x)$'s support is confined within the past and future light cones; it is singular on the light cones themselves (see Greiner & Reinhardt 1996, Section 4.4). It may be checked that both $(\Delta(x-x_0), \partial_t\Delta(x-x_0))$ and $(i\Delta_1(x-x_0), i\partial_t\Delta_1(x-x_0))$ are solutions to the phase-space representation's Schrödinger equation:

$$J\partial_t\left(\Delta(x-x_0), \partial_t\Delta(x-x_0)\right) = A\left(\Delta(x-x_0), \partial_t\Delta(x-x_0)\right); \qquad (155)$$

$$J\partial_t\left(i\Delta_1(x-x_0), i\partial_t\Delta_1(x-x_0)\right) = A\left(i\Delta_1(x-x_0), i\partial_t\Delta_1(x-x_0)\right). \qquad (156)$$

The one-particle state ψ_{x_0} associated with the local field operator $\Phi(x_0) \equiv \Phi(\psi_{x_0})$, in the phase-space representation, is then

$$(\psi_{x_0}(x), \pi_{x_0}(x)) = (i\Delta_1(x-x_0), A\Delta(x-x_0)) = J(\Delta(x-x_0), -iA\Delta_1(x-x_0)). \qquad (157)$$

Newton-Wigner representation
We follow the usual prescription $\psi^{NW}(x) \equiv \sqrt{2}(A^{\frac{1}{2}}\psi^{(+)})(x)$ to obtain

$$\psi^{NW}_{x_0}(x) = \sqrt{2}iA^{\frac{1}{2}}\Delta^{(+)}(x-x_0) =: i\Delta_{NW}(x-x_0) \qquad (158)$$

where we have baptized the *Newton-Wigner free propagator*

$$\Delta_{NW}(x) := -i\int \mathrm{d}^4k\ \sqrt{2k_0}\delta(k_0^2-\omega(\mathbf{k})^2)\Theta(k_0)e^{-ik\cdot x} = -i\int \frac{\mathrm{d}^3\mathbf{k}}{\sqrt{2\omega(\mathbf{k})}}\ e^{-i(\omega(\mathbf{k})t-\mathbf{k}.\mathbf{x})}, \qquad (159)$$

which satisfies the Newton-Wigner representation's Schrödinger equation

$$i\partial_t\Delta_{NW}(x-x_0) = A\Delta_{NW}(x-x_0). \qquad (160)$$

In all representations, any two "local" states ψ_x, ψ_y have the inner product

$$\langle\psi_x, \psi_y\rangle = i\Delta^{(+)}(x-y) = \frac{1}{2}i\Delta_1(x-y) + \frac{1}{2}i\Delta(x-y), \qquad (161)$$

where the last expression separates the inner product into its real and imaginary parts, respectively. And so

$$[\Phi(x), \Phi(y)] = i\Omega(\psi_x, \psi_y) = 2i\Im m\langle\psi_x, \psi_y\rangle = i\Delta(x-y), \qquad (162)$$

which entails commutativity of the local field operators at spacelike separation.

Noncommuting "local" number operators
The fact that position eigenstates don't exist in the one-particle structure, and the consequent fact that we can't create or annihilate localized particles—even though we may interpret $\Phi(x)$ as a genuinely local field operator—, serve to explain an otherwise puzzling fact, namely that apparently "local" number operators fail to commute at spacelike separation. From the fact that the "local" ladder operators $a(x) := a(\psi_x), a^\dagger(x) := a^\dagger(\psi_x)$ satisfy

$$[a(x), a^\dagger(y)] = \langle\psi_x, \psi_y\rangle = i\Delta^{(+)}(x-y), \qquad (163)$$

it follows that (see also Duncan 2012, p. 161)

$$\begin{aligned}
[a^\dagger(x)a(x), a^\dagger(y)a(y)] &= a^\dagger(x)[a(x), a^\dagger(y)a(y)] \;+\; [a^\dagger(x), a^\dagger(y)a(y)]a(x) && (164)\\
&= a^\dagger(x)a^\dagger(y)[a(x), a(y)] \;+\; a^\dagger(x)[a(x), a^\dagger(y)]a(y) \\
&\quad + a^\dagger(y)[a^\dagger(x), a(y)]a(x) \;+\; [a^\dagger(x), a^\dagger(y)]a(y)a(x) && (165)\\
&= i\Delta^{(+)}(x-y)a^\dagger(x)a(y) \;-\; i\Delta^{(+)}(y-x)a^\dagger(y)a(x) && (166)\\
&= i\Delta^{(+)}(x-y)a^\dagger(x)a(y) \;+\; i\Delta^{(-)}(x-y)a^\dagger(y)a(x), && (167)
\end{aligned}$$

and since $\Delta^{(+)}(x)$ and $\Delta^{(-)}(x)$ have spacelike tails, we have apparent interference between particle numbers at spacelike separation (though not for the vacuum state of course, which is an eigenstate of all number operators, associated with eigenvalue zero).

Spacetime localization?
Returning to the local field operators $\Phi(\mathbf{x}, t)$, now explicitly including time-dependence, we find that (where $x := (\mathbf{x}, t)$)

$$\Phi(x) \equiv \Phi(\psi_x) = \Phi\left(\Pi^+(m)\xi_x\right), \tag{168}$$

where we introduce the (improper) *position-time eigenstate* ξ_x, to be associated with the eigenvalue $x = (\mathbf{x}, t)$, and now treat Φ as a function on $\mathcal{H}$ rather than S. We can naturally extend our three representations to investigate the form of ξ_x. In the phase-space representation, this extension leads to

$$\xi_{x_0}(x) = 2\delta^{(4)}(x - x_0); \qquad \pi_{\xi_{x_0}}(x) = \mathbf{0}\ . \tag{169}$$

In the positive-frequency representation, we have

$$\xi^{(+)}_{x_0}(x) = \delta^{(4)}(x - x_0). \tag{170}$$

Both are tantalizing in their elegance! Clearly, the position-time eigenstates take the interpretation suggested by their name in the phase-space and positive-frequency representations. In the Newton-Wigner representation,

$$\xi^{NW}_{x_0}(x) = \sqrt{2}A^{\frac{1}{2}}\delta^{(4)}(x - x_0) = \int \mathrm{d}^4k\ \sqrt{2k_0}e^{-ik\cdot(x-x_0)}. \tag{171}$$

The state $\psi_{(\mathbf{x},t)} \equiv \Pi^{(+)}(m)\xi_x$ is the projection of the position-time eigenstate ξ_x onto the one-particle structure associated with the Hamiltonian $A = \sqrt{\mathbf{P}^2 + m^2}$. We may wonder whether there might be a *spacetime* representation $(\mathfrak{F}_+(\mathcal{H}), W, \Gamma, \nu)$ of the free bosonic field in which $\mathcal{H} = L^2(\mathbb{R}^4)$ and we can make sense of the field operators $\Phi\left(\xi_x\right)$. This possibility will be explored another time.

Newton-Wigner localization
If we adopt the Newton-Wigner standard of localization, with (improper) position eigenstates $\phi_{\mathbf{x}_0}$, then we can make sense of the creation or annihilation of genuinely localized single-particle states. The field operators associated with these ladder operators are (using the positive-

frequency representation)

$$
\begin{aligned}
\Phi^{(NW)}(\mathbf{x}_0) &:= \Phi\left(K_+^{-1}\phi_{\mathbf{x}_0}^{(+)}\right) \;=\; a_{(+)}\left(\phi_{\mathbf{x}_0}^{(+)}\right) + a_{(+)}^{\dagger}\left(\phi_{\mathbf{x}_0}^{(+)}\right) && (172)\\
&= \int \mathrm{d}^3\mathbf{k}\;\left[a_{(+)}\left(\frac{1}{\sqrt{2\omega(\mathbf{k})}}e^{i\mathbf{k}.\mathbf{x}}\right)e^{i\mathbf{k}.\mathbf{x}_0} + a_{(+)}^{\dagger}\left(\frac{1}{\sqrt{2\omega(\mathbf{k})}}e^{i\mathbf{k}.\mathbf{x}}\right)e^{-i\mathbf{k}.\mathbf{x}_0}\right] && (173)\\
&= \int \mathrm{d}^3\mathbf{k}\;\left[a\left(\mathbf{k}\right)e^{i\mathbf{k}.\mathbf{x}_0} + a^{\dagger}\left(\mathbf{k}\right)e^{-i\mathbf{k}.\mathbf{x}_0}\right] && (174)\\
&= \Phi\left(\sqrt{2}A^{\frac{1}{2}}K_+^{-1}\psi_{(\mathbf{x}_0,0)}^{(+)}\right) && (175)\\
&= \sqrt{2}\Gamma\left(A^{\frac{1}{2}}\right)\Phi(\mathbf{x_0},0)\;\Gamma\left(A^{\frac{1}{2}}\right)^{-1} \;=\; \sqrt{2}\left(-\nabla_{\mathbf{x}_0}^2+m^2\right)^{\frac{1}{4}}\Phi(\mathbf{x_0},0). && (176)
\end{aligned}
$$

These field operators also commute at spacelike separation; we use (162) and the fact above that $\Phi^{(NW)}(\mathbf{x})$ and $\Phi(\mathbf{x})$ are related by a unitary transformation. Since local interactions are implemented by polynomials in $\Phi(K^{-1}\psi_x) \neq \Phi(K^{-1}\phi_x)$, interactions cannot be interpreted as strictly local (in space) if we take $\Phi^{(NW)}(\mathbf{x})$ and not $\Phi(\mathbf{x})$ as our local field operators. We'll see this explicitly in the Hamiltonian, below.

The momentum field operators

We can similarly reverse-engineer the momentum field operators $\Pi_\Phi(\mathbf{x},t)$. We find that, in the positive-energy representation (and similarly for the others),

$$
\begin{aligned}
\Pi_\Phi(x_0) &= \partial_t\Phi(x_0) \;=\; -i\int \mathrm{d}^3\mathbf{k}\sqrt{\frac{\omega(\mathbf{k})}{2}}\;\left[a(\mathbf{k})e^{-ik\cdot x_0} - a^{\dagger}(\mathbf{k})e^{ik\cdot x_0}\right]_{k_0=\omega(\mathbf{k})} && (177)\\
&= a_{(+)}\left[iA\int \mathrm{d}^3\mathbf{k}\;\left.\frac{e^{ik\cdot(x-x_0)}}{2\omega(\mathbf{k})}\right|_{k_0=\omega(\mathbf{k})}\right] + a_{(+)}^{\dagger}\left[iA\int \mathrm{d}^3\mathbf{k}\;\left.\frac{e^{-ik\cdot(x-x_0)}}{2\omega(\mathbf{k})}\right|_{k_0=\omega(\mathbf{k})}\right] && (178)\\
&= \Phi\left[K_+^{-1}\left(-A\Delta^{(+)}(x-x_0)\right)\right] && (179)\\
&= \Phi\left[K_+^{-1}\left(iA\psi_{(\mathbf{x}_0,t_0)}^{(+)}(\mathbf{x},t)\right)\right] && (180)\\
&= \Gamma(A)\Phi\left[K_+^{-1}\left(i\psi_{(\mathbf{x}_0,t_0)}^{(+)}(\mathbf{x},t)\right)\right]\Gamma(A)^{-1} && (181)\\
&= \sqrt{-\nabla_{\mathbf{x}_0}^2+m^2}\;\Phi\left[K^{-1}\left(i\psi_{(\mathbf{x}_0,t_0)}\right)\right]. && (182)
\end{aligned}
$$

We may also infer from (180), the definition of the positive-frequency map K_+, and the fact that $\psi_{(\mathbf{x}_0,t_0)}^{(+)}(\mathbf{x},t_0) = \frac{1}{2}A^{-1}\delta^{(3)}(\mathbf{x}-\mathbf{x}_0)$, that

$$
\Pi_\Phi(\mathbf{x}_0) = \Phi\left(\mathbf{0}, A\delta^{(3)}(\mathbf{x}-\mathbf{x}_0)\right), \tag{183}
$$

which we would be led to believe by analogy with the simple harmonic oscillator (for which $P = \Phi(J(1,0)) = \Phi(0, m\omega)$). It may now be checked that

$$
[\Phi(x), \Pi_\Phi(y)] = \partial_{y_0}[\Phi(x),\Phi(y)] = i\partial_{y^0}\Delta(x-y), \tag{184}
$$

so that for $x^0 = y^0 =: t$, we have the familiar equal-time CCRs:

$$
[\Phi(\mathbf{x},t), \Pi_\Phi(\mathbf{y},t)] = i\partial_t\Delta(\mathbf{x}-\mathbf{y},0) = i\delta^{(3)}(\mathbf{x}-\mathbf{y}). \tag{185}
$$

The Newton-Wigner "local" field operators also have associated momentum field operators. These are given by

$$
\begin{aligned}
\Pi_\Phi^{(NW)}(\mathbf{x}_0) &:= \Pi_\Phi(K^{-1}\phi_{\mathbf{x}_0}) = \partial_t\Phi\left(K^{-1}\phi_{\mathbf{x}_0}\right) && (186)\\
&= \Gamma(A)\Phi\left(K^{-1}\left(i\phi_{\mathbf{x}_0}\right)\right)\Gamma(A)^{-1}, && (187)
\end{aligned}
$$

which, it may be checked, are related to the standard momentum field operators $\Pi_\Phi(\mathbf{x}_0, 0)$ by

$$\Pi_\Phi^{(NW)}(\mathbf{x}_0) = \sqrt{2}\Gamma\left(A^{\frac{1}{2}}\right)\Pi_\Phi(\mathbf{x}_0, 0)\Gamma\left(A^{\frac{1}{2}}\right)^{-1}. \tag{188}$$

It is important to note that, according to (176) and (188), the Newton-Wigner "local" field and momentum field operators are related to the standard local field and momentum field operators, respectively, in the same way; viz. by $\Gamma\left(A^{\frac{1}{2}}\right)$. If follows from this that a transformation between the standard local and Newton-Wigner "local" field operators does not mix creation and annihilation operators. The upshot is that the Newton-Wigner vacuum is the same as the standard vacuum, and so (as we would expect) the standard and Newton-Wigner Fock representations are unitarily equivalent. (See Halvorson 2001 for a discussion of some apparent advantages of the Newton-Wigner representation, such as the fact that, for any compact region $G \subset \mathbb{R}^3$, the Fock space factorizes: $\mathfrak{F}_+(L^2(\mathbb{R}^3)) = \mathfrak{F}_+(L^2(G)) \otimes \mathfrak{F}_+(L^2(\overline{G}))$, where $\overline{G}$ is the complement of G.) As we shall below, the same cannot be said for two standard Fock representations associated with different rest masses—precisely due to the fact that the local field operators and momentum field operators transform differently.

The free field Hamiltonian

In terms of momentum ladder operators, we have already seen that the free field Hamiltonian is

$$H = \int \mathrm{d}^3\mathbf{k}\ \omega(\mathbf{k})a^\dagger(\mathbf{k})a(\mathbf{k}). \tag{189}$$

We may re-express H as a function of ladder operators associated with the states $\psi_{\mathbf{x}_0}$. First notice that the momentum eigenstates satisfy

$$\phi_{\mathbf{k}}^{(+)}(\mathbf{x}) = \frac{e^{i\mathbf{k}.\mathbf{x}}}{\sqrt{2\omega(\mathbf{k})}} = \int \mathrm{d}^3\mathbf{y}\ \sqrt{2}i(A^{\frac{1}{2}}\Delta^{(+)})(\mathbf{x}-\mathbf{y}, 0)e^{i\mathbf{k}.\mathbf{y}}. \tag{190}$$

It follows that

$$\begin{aligned}
\sqrt{2\omega(\mathbf{k})}a^\dagger(\mathbf{k}) &= a^\dagger_{(+)}\left(\sqrt{2\omega(\mathbf{k})}\phi_{\mathbf{k}}^{(+)}(\mathbf{x})\right) && (191)\\
&= \int \mathrm{d}^3\mathbf{y}\ a^\dagger_{(+)}\left(2iA\Delta^{(+)}(\mathbf{x}-\mathbf{y}, 0)\right)e^{i\mathbf{k}.\mathbf{y}} && (192)\\
&= \int \mathrm{d}^3\mathbf{y}\ 2\Gamma(A)\,a^\dagger_{(+)}\left(i\Delta^{(+)}(\mathbf{x}-\mathbf{y}, 0)\right)\Gamma(A)^{-1}e^{i\mathbf{k}.\mathbf{y}} && (193)\\
&= \int \mathrm{d}^3\mathbf{y}\ 2\Gamma(A)\,a^\dagger(\mathbf{y})\Gamma(A)^{-1}e^{i\mathbf{k}.\mathbf{y}}, && (194)
\end{aligned}$$

where we use the shorthand $a^\dagger(\mathbf{x}) := a^\dagger_{(+)}\left(\psi_{\mathbf{x}}^{(+)}\right)$. And so

$$\omega(\mathbf{k})a^\dagger(\mathbf{k})a(\mathbf{k}) = \int \mathrm{d}^3\mathbf{x}\int \mathrm{d}^3\mathbf{y}\ 2\Gamma(A)\,a^\dagger(\mathbf{x})a(\mathbf{y})\Gamma(A)^{-1}e^{i\mathbf{k}.(\mathbf{x}-\mathbf{y})}, \tag{195}$$

from which it follows that

$$H = \int \mathrm{d}^3\mathbf{k}\ \omega(\mathbf{k})a^\dagger(\mathbf{k})a(\mathbf{k}) = \int \mathrm{d}^3\mathbf{x}\ 2\Gamma(A)\,a^\dagger(\mathbf{x})a(\mathbf{x})\Gamma(A)^{-1}. \tag{196}$$

We now note that (using (136) and (181))

$$\begin{aligned}
a^\dagger(\mathbf{x}) &= \frac{1}{2}\left[\Phi\left(K_+^{-1}\psi_{\mathbf{x}}^{(+)}\right) - i\Phi\left(K_+^{-1}i\psi_{\mathbf{x}}^{(+)}\right)\right] && (197)\\
&= \frac{1}{2}\left[\Phi(\mathbf{x}) - i\Gamma(A)^{-1}\Pi_\Phi(\mathbf{x})\Gamma(A)\right] && (198)
\end{aligned}$$

to obtain

$$a^\dagger(\mathbf{x})a(\mathbf{x}) = \frac{1}{4} : \Phi(\mathbf{x})^2 + \Gamma(A)^{-1}\Pi_\Phi(\mathbf{x})^2\Gamma(A) : , \tag{199}$$

where we impose normal ordering to avoid an infinite additive constant. By substitution, we obtain

$$H = \int \mathrm{d}^3\mathbf{x} \ : \frac{1}{2}\Pi_\Phi(\mathbf{x})^2 + \frac{1}{2}\Gamma(A)\Phi(\mathbf{x})^2\Gamma\,(A)^{-1} : . \tag{200}$$

But

$$\Gamma(A)\Phi(\mathbf{x})^2\Gamma\,(A)^{-1} = \left(\Gamma(A)\Phi(\mathbf{x})\Gamma\,(A)^{-1}\right)^2 = \Phi\left(K^{-1}(A\psi_\mathbf{x})\right)^2 = \left(\sqrt{-\nabla^2+m^2}\Phi(\mathbf{x})\right)^2, \tag{201}$$

and we use the fact that

$$\int \mathrm{d}^3\mathbf{x} \ \left(\sqrt{-\nabla^2+m^2}\Phi(\mathbf{x})\right)^2 = \int \mathrm{d}^3\mathbf{x} \ \Phi(\mathbf{x})\left(-\nabla^2+m^2\right)\Phi(\mathbf{x}) \tag{202}$$

to finally obtain the familiar expression

$$H = \int \mathrm{d}^3\mathbf{x} \ : \frac{1}{2}\Pi_\Phi(\mathbf{x})^2 - \frac{1}{2}\Phi(\mathbf{x})\nabla^2\Phi(\mathbf{x}) + \frac{1}{2}m^2\Phi(\mathbf{x})^2 : . \tag{203}$$

The equation of motion for the quantum field $|\Psi\rangle(t)$ is given, as usual, by

$$|\Psi\rangle(t) = e^{-i\int_0^t \mathrm{d}t H}|\Psi\rangle(0) = e^{-i\int_{[0,t]\times\mathbb{R}^3}\mathrm{d}^4x\mathcal{H}(x)}|\Psi\rangle(0), \tag{204}$$

where the *Hamiltonian density* $\mathcal{H}(x)$ is defined as

$$\mathcal{H}(x) := : \frac{1}{2}\Pi_\Phi(x)^2 - \frac{1}{2}\Phi(x)\nabla^2\Phi(x) + \frac{1}{2}m^2\Phi(x)^2 : . \tag{205}$$

We can also express the Hamiltonian in terms of the Newton-Wigner "local" field and momentum field operators. We find, using (176), (188) and (200), that

$$\begin{aligned} H &= \int \mathrm{d}^3\mathbf{x} \ \frac{1}{4} : \Gamma(A^{\frac{1}{2}})^{-1}\Pi_\Phi^{(NW)}(\mathbf{x})^2\Gamma(A^{\frac{1}{2}}) \ + \ \Gamma(A^{\frac{1}{2}})\Phi^{(NW)}(\mathbf{x})^2\Gamma(A^{\frac{1}{2}})^{-1} : & (206)\\ &= \int \mathrm{d}^3\mathbf{x} \ \frac{1}{4} : \Pi_\Phi^{(NW)}(\mathbf{x})\frac{1}{\sqrt{-\nabla^2+m^2}}\Pi_\Phi^{(NW)}(\mathbf{x}) \ + \ \Phi^{(NW)}(\mathbf{x})\sqrt{-\nabla^2+m^2}\Phi^{(NW)}(\mathbf{x}) : , & (207)\end{aligned}$$

both terms of which describe interactions which are nonlocal according to the Newton-Wigner standard of localization. This is down to $A^{\frac{1}{2}}$ and $A^{-\frac{1}{2}}$ both being anti-local operators.

5.8 Inequivalent representations

Unitarily inequivalent representations arise from two sources: choosing a different vacuum state and imposing a different dynamics.

Alternative choices for the vacuum

Choose any orthonormal basis $\{\xi_i\}$ for the one-particle structure $\mathcal{H}$. Then the vacuum ν chosen above satisfies, for all i,

$$\mathrm{d}\Gamma(\Pi(\xi_i))\nu = a^\dagger(\xi_i)a(\xi_i)\nu = 0; \tag{208}$$

i.e. we have no particles in any state. We can write ν in terms of occupation numbers for the ξ_i:

$$\nu = |0_1, 0_2, 0_3, \ldots\rangle, \tag{209}$$

where '0_i' indicates that $d\Gamma(\Pi(\xi_i))\nu = 0$. The expression (209) suggests $\aleph_0^{\aleph_0}$ = continuum-many alternative states, each one specified by a function from natural numbers (labelling independent modes) to natural numbers (giving the occupation number of that mode). Yet we know that the Fock space $\mathfrak{F}_+(\mathcal{H})$ is separable, i.e. has a countable basis. So (like the infinite spin-chain), we expect that we can only represent (superpositions of) states that each involve finitely many excitations from an appropriate ground state.

One might suggest that an alternative "vacuum" ν' could be defined by choosing a natural number $n \in \mathbb{N}$ and taking a state with n excitations in every mode to be stipulated as the new vacuum or ground state. So we write

$$\nu' := |n_1, n_2, n_3, \ldots\rangle. \tag{210}$$

This suggestion is "hairy": there are issues about normalization, for a start; and we also have to define rather strange ladder operators such that $a(\xi_i)\nu' = 0$. But the idea will be that any state accessible from ν' with arbitrarily many finite applications of ladder operators will remain orthogonal to ν—indeed orthogonal to any state in the usual Fock space defined above. Therefore the Fock space defined on ν' provides a representation which is disjoint from the Fock space defined on ν.

There is, however, a standard analysis (e.g. Greiner and Reinhardt (1996), Example 1.2, pp. 10-26) of how perturbing a system of uncoupled harmonic oscillators can yield a ground-state for the perturbed system that is a coherent state when expressed in terms of the original Fock space. This leads in to the second source of inequivalent representations ...

Alternative dynamics

The fact that the field with nontrivial dynamics cannot be represented in the corresponding free field's Fock space is the upshot of *Haag's Theorem*; but we needn't even consider nontrivial dynamics here. Consider instead a simple change in the single particle's rest mass $m_1 \mapsto m_2$ (see Duncan 2012, SEction 10.5). In the one-particle structure, this corresponds to a change in the single-particle Hamiltonian:

$$A_1 := \sqrt{-\nabla^2 + m_1^2} \qquad \mapsto \qquad A_2 := \sqrt{-\nabla^2 + m_2^2}, \tag{211}$$

which, we might think, in analogy with the simple harmonic oscillator, may be implemented in the field theory by the transformations

$$\begin{aligned} \Phi(\mathbf{x}) &\mapsto \Gamma\left(A_2^{\frac{1}{2}} A_1^{-\frac{1}{2}}\right) \Phi(\mathbf{x}) \Gamma\left(A_2^{\frac{1}{2}} A_1^{-\frac{1}{2}}\right)^{-1}; \\ \Pi_\Phi(\mathbf{x}) &\mapsto \Gamma\left(A_2^{\frac{1}{2}} A_1^{-\frac{1}{2}}\right)^{-1} \Pi_\Phi(\mathbf{x}) \Gamma\left(A_2^{\frac{1}{2}} A_1^{-\frac{1}{2}}\right). \end{aligned} \tag{212}$$

This leads to the new momentum ladder operators

$$a_2(\mathbf{k}) = \frac{1}{2}\left(\sqrt{\frac{\omega_2(\mathbf{k})}{\omega_1(\mathbf{k})}} + \sqrt{\frac{\omega_1(\mathbf{k})}{\omega_2(\mathbf{k})}}\right) a_1(\mathbf{k}) + \frac{1}{2}\left(\sqrt{\frac{\omega_2(\mathbf{k})}{\omega_1(\mathbf{k})}} - \sqrt{\frac{\omega_1(\mathbf{k})}{\omega_2(\mathbf{k})}}\right) a_1^\dagger(\mathbf{k}); \tag{213}$$

$$a_2^\dagger(\mathbf{k}) = \frac{1}{2}\left(\sqrt{\frac{\omega_2(\mathbf{k})}{\omega_1(\mathbf{k})}} - \sqrt{\frac{\omega_1(\mathbf{k})}{\omega_2(\mathbf{k})}}\right) a_1(\mathbf{k}) + \frac{1}{2}\left(\sqrt{\frac{\omega_2(\mathbf{k})}{\omega_1(\mathbf{k})}} + \sqrt{\frac{\omega_1(\mathbf{k})}{\omega_2(\mathbf{k})}}\right) a_1^\dagger(\mathbf{k}). \tag{214}$$

Clearly, the vacuum ν_1 for the $a_1(\mathbf{k}), a_1^\dagger(\mathbf{k})$ is not a vacuum for the $a_2(\mathbf{k}), a_2^\dagger(\mathbf{k})$, since $a_2(\mathbf{k})\nu_1 \neq 0$ for all $\mathbf{k}$. In fact, we are led to believe that the first vacuum ν_1 contains *infinitely many* of the particles associated with the second vacuum ν_2, and *vice versa*. We find that

$$\langle \nu_1, d\Gamma_2(\mathbf{k})\nu_1 \rangle = \frac{(\omega_1(\mathbf{k}) - \omega_2(\mathbf{k}))^2}{4\omega_1(\mathbf{k})\omega_2(\mathbf{k})} \delta^{(3)}(\mathbf{0}). \tag{215}$$

The factor $\delta^{(3)}(\mathbf{0})$ is due to our using ladder operators of improper eigenfunctions; by putting the field in a box and imposing periodic boundary conditions, this factor becomes L^3, the volume of the box. But still this entails that

$$\langle \nu_1, H_2 \nu_1 \rangle = \sum_{\mathbf{k} \in \frac{\pi}{L}\mathbb{Z}^3} \omega_2(\mathbf{k}) \langle \nu_1, \mathrm{d}\Gamma_2(\mathbf{k}) \nu_1 \rangle = L^3 \sum_{\mathbf{k} \in \frac{\pi}{L}\mathbb{Z}^3} \frac{(\omega_1(\mathbf{k}) - \omega_2(\mathbf{k}))^2}{4\omega_1(\mathbf{k})} = \infty, \tag{216}$$

even for finite L. In perturbation theory, this is expressed by an ultraviolet divergence in the contribution provided by $H_2 - H_1 = \frac{1}{2}(m_2^2 - m_1^2) \int \mathrm{d}^3\mathbf{x}\ \Phi(\mathbf{x})^2$ to the ν_1-to-ν_1 vacuum transition. (These show up in the Feynman path integral as a divergent series of bubble diagrams.) But all states accessible from ν_1 and all states accessible from ν_2 have finite energy (albeit arbitrarily large). Therefore we must conclude that ν_1 and ν_2 belong to disjoint representations.

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