Mathematical Introduction to Quantum Field Theory

Jan Dereziński
Dept. of Math. Methods in Phys.,
Faculty of Physics, University of Warsaw
Pasteura 5, 02-093 Warszawa, Poland
email Jan.Derezinski@fuw.edu.pl

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Lasciate ogni speranza, voi ch' intrate. (Dante Aligheri, Commedia Divina)

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1 Minkowski space

1.1 Coordinates in Minkowski space

By definition, the *Minkowski space*, denoted $\mathbb{R}^{1,n}$, is the vector space $\mathbb{R}^{1+n}$ equipped with the canonical pseudo-Euclidean form of signature $(-+\cdots+)$. Its coordinates will be typically denoted by x^μ, $\mu = 0, 1, \ldots, n$. The pseudo-Euclidean form is then given by

$$g_{\mu\nu}x^\mu x^\nu = -(x^0)^2 + \sum_{i=1}^{n}(x^i)^2. \tag{1.1}$$

(Throughout these notes the velocity of light has the value 1 and we use the *Einstein summation convention*). We use the *metric tensor* $[g_{\mu\nu}]$ to lower indices and its inverse $[g^{\mu\nu}]$ to raise indices:

$$x_\mu = g_{\mu\nu}x^\nu, \quad x^\mu = g^{\mu\nu}x_\nu.$$

For a function $\mathbb{R}^{1,n} \ni x \mapsto f(x)$, we will sometimes use various kind of notation for partial derivatives:

$$\frac{\partial f(x)}{\partial x^\mu} = \partial_{x^\mu} f(x) = \partial_\mu f(x) = f_{,\mu}(x).$$

Writing $\mathbb{R}^n$ we will typically denote the *spatial part* of the Minkowski space obtained by setting $x^0 = 0$. If $x \in \mathbb{R}^{1,n}$, then $\vec{x}$ will denote the projection of x onto $\mathbb{R}^n$. Latin letters i, j, k will sometimes denote the spatial indices of a vector. Note that $x_i = x^i$.

On $\mathbb{R}^{1,n}$ we have the standard Lebesgue measure denoted $\mathrm{d}x$. The notation $\mathrm{d}\vec{x}$ will be used for the Lebesgue measure on $\mathbb{R}^n \subset \mathbb{R}^{1,n}$.

We will often write t for $x^0 = -x_0$. The time derivative will be often denoted by a dot:

$$\dot{f}(t) = \frac{\partial f(t)}{\partial t} = \partial_t f(t) = \frac{\partial f(x^0)}{\partial x^0} = \partial_0 f(x^0) = f_{,0}(x^0).$$

1.2 Causal structure

A nonzero vector $x \in \mathbb{R}^{1,n}$ is called

$$\begin{aligned} \textit{timelike} \quad &\text{if} \quad x_\mu x^\mu < 0, \\ \textit{causal} \quad &\text{if} \quad x_\mu x^\mu \le 0, \\ \textit{lightlike} \quad &\text{if} \quad x_\mu x^\mu = 0, \\ \textit{spacelike} \quad &\text{if} \quad x_\mu x^\mu > 0. \end{aligned}$$

A causal vector x is called

$$\begin{aligned} \textit{future oriented} \quad &\text{if} \quad x^0 > 0, \\ \textit{past oriented} \quad &\text{if} \quad x^0 < 0. \end{aligned}$$

The set of future/past oriented causal vectors is called the *future/past light cone* and denoted $J^\pm$. We set $J := J^+ \cup J^-$.

If $\mathcal{O} \subset \mathbb{R}^{1,n}$, its *causal shadow* is defined as $J(\mathcal{O}) := \mathcal{O} + J$. We also define its *future/past shadow* $J^\pm(\mathcal{O}) := \mathcal{O} + J^\pm$.

Lemma 1.1. *Let $\mathcal{O}_i \subset \mathbb{R}^{1,n}$, $i = 1, 2$. Then*

$$J^+(\mathcal{O}_1) \cap \mathcal{O}_2 = \emptyset \;\Leftrightarrow\; \mathcal{O}_1 \cap J^-(\mathcal{O}_2) = \emptyset, \tag{1.2}$$

$$J(\mathcal{O}_1) \cap \mathcal{O}_2 = \emptyset \;\Leftrightarrow\; \mathcal{O}_1 \cap J(\mathcal{O}_2) = \emptyset. \tag{1.3}$$

We will write $\mathcal{O}_1 \times \mathcal{O}_2$ iff (1.3) holds. We then say that $\mathcal{O}_1$ and $\mathcal{O}_2$ are *spatially separated.*

1.3 Lorentz and Poincaré groups

The pseudo-Euclidean group $O(1, n)$ is called the *full Lorentz group.* Its connected component of unity is denoted $SO_0(1, n)$ and called the *connected* or *proper Lorentz group.*

$\Lambda \in O(1, n)$ if for any vector $[x^\mu] \in \mathbb{R}^{1,n}$

$$g_{\mu\nu} x^\mu x^\nu = g_{\alpha\beta} \Lambda^\alpha_\mu x^\mu \Lambda^\beta_\nu x^\nu. \tag{1.4}$$

The full Lorentz group contains special elements: the time reversal T and the space inversion (the parity) P and the space-time inversion X := PT:

$$\mathrm{T}(x^0, \vec{x}) = (-x^0, \vec{x}), \quad \mathrm{P}(x^0, \vec{x}) = (x^0, -\vec{x}), \quad \mathrm{X}x = -x.$$

It consists of four connected components

$$SO_0(1, n),\ \mathrm{T}{\cdot}SO_0(1, n),\ \mathrm{P}{\cdot}SO_0(1, n),\ \mathrm{X}{\cdot}SO_0(1, n).$$

$O(1, n)$ has three subgroups of index two:

$$SO_0(1, n) \cup \mathrm{X}{\cdot}SO_0(1, n), \tag{1.5}$$

$$SO_0(1, n) \cup \mathrm{P}{\cdot}SO_0(1, n), \tag{1.6}$$

$$SO_0(1, n) \cup \mathrm{T}{\cdot}SO_0(1, n). \tag{1.7}$$

(1.5) coincides with $SO(1,n)$ for even $1+n$ and (1.6) coincides with $SO(1,n)$ for odd $1+n$.

The affine extension of the full Lorentz group $\mathbb{R}^{1,n} \rtimes O(1,n)$ is called the *full Poincaré group*. Its elements will be typically written as (y,Λ). On $x \in \mathbb{R}^{1,n}$ it acts by

$$(y,\Lambda)x := y + \Lambda x.$$

Here is the multiplication:

$$(y_1,\Lambda_1)(y_2+\Lambda) = (y_1 + \Lambda_1 y_2, \Lambda_1\Lambda_2). \tag{1.8}$$

We will often write y instead of $(y,\mathbb{1})$ and Λ instead of $(0,\Lambda)$. It is the full symmetry group of the Minkowski space.

Example 1.2. *Let us determine $O(1,1)$. We set*

$$x_+ := x+t, \quad x_- := x-t; \quad x = \frac{1}{2}(x_+ + x_-), \quad t = \frac{1}{2}(x_+ - x_-).$$

Now, let $A = \begin{bmatrix} a & b \\ c & d \end{bmatrix}$.

$$x^2 - t^2 = x_- x_+ = (ax_+ + bx_-)(cx_+ + dx_-)$$

is solved by

$$ad + bc = 1, \quad ac = 0, \quad bd = 0.$$

This has 4 types of solutions:

$$a > 0, \quad d > 0, \quad b = c = 0, \tag{1.9}$$
$$a < 0, \quad d < 0, \quad b = c = 0, \tag{1.10}$$
$$b > 0, \quad c > 0, \quad a = d = 0, \tag{1.11}$$
$$b > 0, \quad c > 0, \quad a = d = 0. \tag{1.12}$$

Finally, we set

$$A = \frac{1}{2}\begin{bmatrix} 1 & -1 \\ 1 & 1 \end{bmatrix}\begin{bmatrix} a & b \\ c & d \end{bmatrix}\begin{bmatrix} 1 & 1 \\ -1 & 1 \end{bmatrix}.$$

1.4 Euclidean space

We will sometimes consider the Euclidean space $\mathbb{R}^d$ equipped with the form

$$|x|^2 = (x^1)^2 + \cdots (x^d)^2. \tag{1.13}$$

The orthogonal group $O(d)$ has only two connected components, one of them is the group $SO(d)$. We also have the Euclidean group $\mathbb{R}^d \rtimes O(d)$.

Note that if $d = 1+n$ and we set $x^0 = \pm \mathrm{i} x^d$, then (1.13) becomes the Minkowski form (1.1). This trick is called the *Wick rotation.*

1.5 Joint spectrum

Assume first that $\mathcal{H}$ is a finite dimensional Hilbert space. The spectrum of an operator A then is defined as the set of its eigenvalues.

We say that A is self-adjoint if $A = A^*$. The spectral theorem says that if A is self-adjoint, then

$$A = \sum_{a \in \mathrm{sp}(A)} a \mathbb{1}_a(A). \tag{1.14}$$

where $\mathbb{1}_a(A)$ is the orthogonal projection onto eigenvectors of A with eigenvalue a. More generally, if $\Omega \subset \mathrm{sp}(A)$, then we set

$$\mathbb{1}_\Omega(A) := \sum_{a \in \Omega} \mathbb{1}_a(A).$$

Let self-adjoint operators $A_1, \ldots, A_n$ commute. Then so do their spectral projections. Define the *joint spectrum* of $A_1, \ldots, A_n$ by

$$\mathrm{sp}(A_1, \ldots, A_n) := \{(a_1, \ldots, a_n) \in \mathbb{R}^n \ : \ \mathbb{1}_{\{a_1\}}(A_1) \cdots \mathbb{1}_{\{a_n\}}(A_n) \neq 0.\}.$$

For any subset $\Omega \subset \mathrm{sp}(A_1, \ldots, A_n)$ we define the *spectral projection of* $A_1, \ldots, A_n$ *onto* Ω:

$$\mathbb{1}_\Omega(A_1, \ldots A_n) := \sum_{(a_1, \ldots, a_n) \in \Omega} \mathbb{1}_{\{a_1\}}(A_1) \cdots \mathbb{1}_{\{a_n\}}(A_n).$$

Assume now that $\mathcal{H}$ is a Hilbert space of any dimension. The spectrum of an operator A is defined as

$$\mathrm{sp}(A) := \{z \in \mathbb{C} \mid (z - A)^{-1} \text{ does not exist}\}.$$

The set of eigenvalues of A is called the *point spectrum of* A and is contained in $\mathrm{sp}(A)$

The spectral theorem says that if A is self-adjoint, then we can define for any Borel set $\Omega \subset \mathrm{sp}(A)$ the corresponding spectral projection, denoted $\mathbb{1}_\Omega(A)$. They are orthogonal projections. They satisfy

$$\mathbb{1}_{\Omega_1}(A) \mathbb{1}_{\Omega_2}(A) = \mathbb{1}_{\Omega_1 \cap \Omega_2}(A). \tag{1.15}$$

Let $A_1, \ldots, A_n$ be self-adjoint operators that strongly commute, that is their spectral projections commute. We say that $(a_1, \ldots, a_n) \in \mathrm{sp}(A_1, \ldots, A_n)$ if for any $\epsilon > 0$

$$\mathbb{1}_{[a_1 - \epsilon, a_1 + \epsilon]}(A_1) \cdots \mathbb{1}_{[a_n - \epsilon, a_n + \epsilon]}(A_n) \neq 0. \tag{1.16}$$

Clearly

$$\mathrm{sp}(A_1, \ldots, A_n) \subset \mathrm{sp}(A_1) \times \cdots \times \mathrm{sp}(A_n), \tag{1.17}$$

$$\mathrm{sp}(UA_1U^{-1}, \ldots, UA_nU^{-1}) = \mathrm{sp}(A_1, \ldots, A_n) \tag{1.18}$$

Example 1.3. *Consider the commuting self-adjoint operators* $L^2 = L_x^2 + L_y^2 + L_z^2$ *and* L_z*.*

$$\mathrm{sp}(L^2) = \{\ell(\ell+1) \mid \ell = 0, 1, \dots\} \tag{1.19}$$

$$\mathrm{sp}(L_z) = \mathbb{Z}, \tag{1.20}$$

$$\mathrm{sp}(L^2, L_z) = \big\{\big(\ell(\ell+1), m\big) \mid \ell = 0, 1, \dots;\ m = -\ell, -\ell+1, \dots, \ell\big\}. \tag{1.21}$$

Example 1.4. *Consider* $p_j = -\mathrm{i}\partial_{x^j}$, $-\Delta = \sum_{j=1}^d p_j^2$*. They are commuting self-adjoint operators.*

$$\mathrm{sp}(p_j) = \mathbb{R}; \tag{1.22}$$

$$\mathrm{sp}(-\Delta) = [0, \infty[\tag{1.23}$$

$$\mathrm{sp}(p_1, p_2, p_3, -\Delta) = \{(k_1, k_2, k_3, k_1^2 + k_2^2 + k_3^2 \mid k_1, k_2, k_3 \in \mathbb{R}\}. \tag{1.24}$$

This follows from

$$(\mathcal{F}^{-1} p_j \mathcal{F} f)(k) = k_j f(k). \tag{1.25}$$

1.6 Quantum mechanics

Pure quantum states are described by normalized vectors in a Hilbert space $\mathcal{H}$. The dynamics is usually described by considering a strongly continuous 1-parameter unitary group on $\mathcal{H}$, that is, a strongly continuous function $\mathbb{R} \ni t \mapsto U(t) \in U(\mathcal{H})$ such that

$$U(t_1)U(t_2) = U(t_1 + t_2), \quad t_1, t_2 \in \mathbb{R},$$

The *Stone Theorem* says that $U(t) := \mathrm{e}^{-\mathrm{i}tH}$ for a uniquely defined self-adjoint operator H, called a *Hamiltonian*.

In typical situations the *Hamiltonian* is bounded from below, which means that there exists $E \in \mathbb{R}$ such that

$$(f|Hf) \geq E(f|f), f \in \mathcal{H}. \tag{1.26}$$

Equivalently, $\mathrm{sp}(H) \subset [E, \infty[$. It does not affect any physical predictions if we subtract from the Hamiltonian the infimum of its spectrum.

The Hamiltonian has often a ground state, that means $\inf \mathrm{sp}(H)$ is an eigenvalue. The ground state is often nondegenerate.

It will be convenient to formalize these properties.

Definition 1.5. *We will say that* $\mathcal{H}, H, \Omega$ *satisfy the* standard requirements of quantum mechanics (QM) *if*

(1) $\mathcal{H}$ *is a Hilbert space;*

(2) H *is a positive self-adjoint operator on* $\mathcal{H}$ *(called the Hamiltonian);*

(3) Ω *is a normalized eigenvector of* H *with eigenvalue* 0*;*

(4) Ω *is nondegenerate as an eigenvector of* H*.*

1.7 Relativistic quantum mechanics

Let us assume that there are no fermions. Relativistic covariance of a quantum system described by a Hilbert space $\mathcal{H}$ is expressed by choosing a strongly continuous unitary representation of the connected Poincaré group

$$\mathbb{R}^{1,3} \rtimes SO_0(1,3) \ni (y,\Lambda) \mapsto U(y,\Lambda) \in U(\mathcal{H}). \tag{1.27}$$

We will denote the self-adjoint generator of space-time translations by $P = (P^0, \vec{P})$. $P^0 = H$ is the *Hamiltonian*. $\vec{P}$ is called the *momentum*. Thus

$$U((t,\vec{y}),\mathbb{1}) = \mathrm{e}^{-\mathrm{i}tH+\mathrm{i}\vec{y}\vec{P}}.$$

(We assume that the Planck constant $\hbar$ equals 1).

Proposition 1.6. $\mathrm{sp}(P)$ *is invariant wrt* $SO_0(1,n)$.

Proof. We compute for $\Lambda \in SO_0(1,n)$:

$$U(\Lambda)\mathrm{e}^{\mathrm{i}xP}U(\Lambda)^{-1} = U(0,\Lambda)U(x,1)U(0,\Lambda^{-1}) \tag{1.28}$$

$$= U(\Lambda x,1) = \mathrm{e}^{\mathrm{i}(\Lambda x)P} = \mathrm{e}^{\mathrm{i}x\Lambda^{\mathrm{T}}P}. \tag{1.29}$$

Differentiating wrt x we obtain

$$U(\Lambda)PU(\Lambda)^{-1} = \Lambda^{\mathrm{T}}P. \tag{1.30}$$

Hence $\Lambda^{\mathrm{T}}\mathrm{sp}(P) = \mathrm{sp}(P)$.

Let us show that

$$SO_0(1,n) = \{\Lambda^{\mathrm{T}} \mid \Lambda \in SO_0(1,n)\}. \tag{1.31}$$

Note that $g = g^{-1}$ (which is valid in the standard coordinates). Using this we check that

$$\Lambda^{\mathrm{T}}g\Lambda = g \;\Rightarrow\; \Lambda g\Lambda^{\mathrm{T}} = g. \tag{1.32}$$

Besides, both sides of (1.31) contain $\mathbb{1}$ and $\Lambda \mapsto \Lambda^{\mathrm{T}}$ is continuous. □

Definition 1.7. *Suppose a representation of the proper Poincaré group is given. The following conditions will be called the* basic requirements of relativistic quantum mechanics (RQM)*:*

(1) Existence of a Poincaré invariant vacuum*: There exists a (normalized) vector* Ω *invariant with respect to* $\mathbb{R}^{1,3} \rtimes SO_0(1,3)$.

(2) Spectral condition*: The joint spectrum of the energy-momentum operator is contained in the forward light cone, that is,* $\mathrm{sp}(P) \subset J^+$.

(3) Uniqueness of the vacuum*: The vector* Ω *is unique up to a phase factor.*

Note that conditions (1)-(3) imply the standard requirements of QM.

More precisely, (2) implies $H \geq 0$. (1) and (2) imply that Ω is the *ground state of* H. (3) implies that this ground state is unique.

Conversely, the Poincaré invariance of $\mathrm{sp}(P)$ and the boundedness from below of H in any system of coordinates imply (2).

2 Algebras and axioms

2.1 States and observables

Let us describe basic framework of quantum mechanics. To avoid technical complications, in the first part of this section we will assume that the Hilbert space $\mathcal{H}$ describing a quantum system is finite dimensional, so that it can be identified with $\mathbb{C}^N$, for some N.

In basic courses on Quantum Mechanics we learn that a quantum state is described by a *density matrix* ρ and a *yes/no experiment* by an *orthogonal projection* P. The probability of the affirmative outcome of such an experiment equals

$$\mathrm{Tr}(\rho P).$$

Two orthogonal projections P_1 and P_2 are simultaneously measurable iff they commute.

We say that a family of orthogonal projections $P_1, \ldots, P_n$ is an *orthogonal partition of unity on* $\mathcal{H}$ iff

$$\sum_{i=1}^{n} P_i = \mathbb{1}, \quad P_i P_j = \delta_{ij} P_j, \quad i, j = 1, \ldots n.$$

Clearly, all elements of an orthogonal partition of unity commute with one another. Therefore, in principle, one can design an experiment that measures simultaneously all of them.

If $P_1, \ldots, P_n$ is an orthogonal partition of unity, then setting $\mathcal{H}_i := \mathrm{Ran} P_i$, $i = 1, \ldots, n$, we obtain an *orthogonal direct sum decomposition* $\mathcal{H} = \bigoplus_{i=1}^{n} \mathcal{H}_i$. Thus specifying an ortogonal partition of unity is equivalnt to speciifying an orthogonal direct sum decomposition.

To any *self-adjoint operator* A we can associate an orthogonal partition of unity given by the *spectral projections of* A *onto its eigenvalues*:

$$\mathbb{1}_{\{a\}}(A), \quad a \in \mathrm{sp}(A). \tag{2.1}$$

By *measuring the observable* A we mean measuring the partition of unity (2.1). Clearly, $A = \sum_{a \in \mathrm{sp}(A)} a \mathbb{1}_a(A)$. Hence, the average eigenvalue of A in such an experiment equals

$$\mathrm{Tr}\rho A = \sum_{a \in \mathrm{sp}(A)} a \mathrm{Tr}\rho \mathbb{1}_a(A). \tag{2.2}$$

We call (2.2) the *expectation value of the observable* A *in the state* ρ.

2.2 Superselection sectors

So far we assumed that all orthogonal projections on $\mathcal{H}$, hence all self-adjoint operators on $\mathcal{H}$, correspond to possible experiments. We say that all self-adjoint elements of $B(\mathcal{H})$ are *observable*.

Sometimes this is not the case. We are going to describe several situations where only a part of self-adjoint operators are observable.

It may happen that the Hilbert space $\mathcal{H}$ has a distinguished direct sum decomposition

$$\mathcal{H} = \bigoplus_{i=1}^{n} \mathcal{H}_n \tag{2.3}$$

such that only self-adjoint operators that preserve each subspace $\mathcal{H}_i$ are measurable. We say then that $\mathcal{H}_i$, $i = 1, \ldots, n$, are *superselection sectors*.

Let Q_i denote the orthogonal projection onto $\mathcal{H}_i$. Then linear combinations of Q_i can be measured simultaneously with all other observables. We say that they are *classical observables*.

If we choose an o.n. basis of $\mathcal{H}$ compatible with (2.3), then only block diagonal self-adjoint matrices are observable. States are also described by block diagonal matrices.

Superselection sectors arise typically when we have a strictly conserved quantity, this means a self-adjoint operator Q that commutes with all possible dynamics. For instance, the *total charge* of the system usually determines a superselection sector. Another example of a superselection sector is the *fermionic parity*: states of an *even* and *odd number of fermions* form two superselection sectors.

2.3 Composite quantum systems

Suppose that two quantum systems are described by Hilbert spaces $\mathcal{H}_1$, $\mathcal{H}_2$. Then the *composite system* is described by the tensor product $\mathcal{H}_1 \otimes \mathcal{H}_2$. Observables of the first system are described by self-adjoint elemens of $B(\mathcal{H}_1) \otimes \mathbb{1}_{\mathcal{H}_2}$, whereas observables of the second system are described by self-adjoint elements of $\mathbb{1}_{\mathcal{H}_1} \otimes B(\mathcal{H}_2)$. Note that they commute, so that one can simultaneously measure them. From the point of view of the first system only self-adjoint elements of $B(\mathcal{H}_1) \otimes \mathbb{1}_{\mathcal{H}_2}$ are observable. Again, we have a situation where not all self-adjoint elements of $B(\mathcal{H})$ are observable.

Let $\mathcal{H}_1 = \mathbb{C}^p$ with an o.n. basis $e_1, \ldots, e_p$ and $\mathcal{H}_2 = \mathbb{C}^q$ with an o.n. basis $f_1, \ldots, f_q$. Then $e_i \otimes f_j$ $i = 1, \ldots, p$, $j = 1, \ldots, q$ is an o.n. basis of $\mathcal{H}_1 \otimes \mathcal{H}_2$. Matrices in $B(\mathbb{C}^p) \otimes \mathbb{1}_{\mathbb{C}^q}$ have the form

$$\begin{bmatrix} A & 0 & & \\ 0 & A & & \\ & & & \\ & & & A \end{bmatrix}, \quad A \in B(\mathbb{C}^p),$$

and matrices in $\mathbb{1}_{\mathcal{H}_1} \otimes B(\mathcal{H}_2)$ have the form

$$\begin{bmatrix} b_{11}\mathbb{1} & b_{12}\mathbb{1} & & \\ b_{21}\mathbb{1} & b_{22}\mathbb{1} & & \\ & & & \\ & & & b_{qq}\mathbb{1} \end{bmatrix}, \quad [b_{ij}] \in B(\mathbb{C}^q),$$

2.4 $*$-algebras

Consider the Hilbert space $\mathcal{H} = \mathbb{C}^N$, $N = \sum_{i=1}^{n} p_i q_i$,

$$\mathcal{H} = \bigoplus_{i=1}^{n} \mathbb{C}^{p_i} \otimes \mathbb{C}^{q_i},$$

and the set

$$\mathfrak{A} := \bigoplus_{i=1}^{n} B(\mathbb{C}^{p_i}) \otimes \mathbb{1}_{q_i}.$$

Note that $\mathfrak{A}$ is a vector space closed wrt the multiplication and the Hermitian conjugation. It is an example of what mathematicians call a $*$-*algebra*, which we recall below.

As discussed before, in the finite dimensional case, observables of a quantum system are described by the self-adjoint part of a certain $*$-subalgebra of $B(\mathcal{H})$.

Let $\mathfrak{A}$ be a vector space over $\mathbb{C}$. We say that $\mathfrak{A}$ is an *algebra* if it is equipped with an operation

$$\mathfrak{A} \times \mathfrak{A} \ni (A, B) \mapsto AB \in \mathfrak{A}$$

satisfying

$$\begin{array}{l} A(B+C) = AB + AC, \quad (B+C)A = BA + CA, \\ (\alpha\beta)(AB) = (\alpha A)(\beta B). \end{array}$$

If in addition

$$A(BC) = (AB)C,$$

we say that it is an *associative algebra*. (In practice by an algebra we will usually mean an associative algebra).

The *center* of an algebra $\mathfrak{A}$ equals

$$\mathfrak{Z}(\mathfrak{A}) = \{A \in \mathfrak{A} \ : \ AB = BA, \ B \in \mathfrak{A}\}.$$

Let $\mathfrak{A}$, $\mathfrak{B}$ be algebras. A map $\phi : \mathfrak{A} \to \mathfrak{B}$ is called a *homomorphism* if it is linear and preserves the multiplication, ie.

(1) $\phi(\lambda A) = \lambda\phi(A)$;

(2) $\phi(A + B) = \phi(A) + \phi(B)$;

(3) $\phi(AB) = \phi(A)\phi(B)$.

We say that an algebra $\mathfrak{A}$ is a $*$-*algebra* if it is equipped with an antilinear map $\mathfrak{A} \ni A \mapsto A^* \in \mathfrak{A}$ such that $(AB)^* = B^*A^*$, $A^{**} = A$ and $A \neq 0$ implies $A^*A \neq 0$.

If $\mathcal{H}$ is a Hilbert space, then $B(\mathcal{H})$ equipped with the hermitian conjugation is a $*$-algebra

If $\mathfrak{A}$, $\mathfrak{B}$ are $*$-algebras, then a homomorphism $\pi : \mathfrak{A} \to \mathfrak{B}$ satisfying $\pi(A^*) = \pi(A)^*$ is called a $*$-*homomorphism*.

Theorem 2.1. (1) *Every finite dimensional $*$-algebra $\mathfrak{A}$ is $*$-isomorphic to*

$$\bigoplus_{i=1}^{n} B(\mathbb{C}^{p_i}),$$

for some $p_1, \dots, p_n$

(2) *If in addition $\mathfrak{A}$ is a subalgebra of $B(\mathbb{C}^N)$ and contains the identity on $\mathbb{C}^N$, then there exist $q_1, \dots, q_n$ with $N = \sum_{i=1}^{n} p_i q_i$, and a basis of $\mathbb{C}^N$ such that*

$$\mathfrak{A} = \bigoplus_{i=1}^{n} B(\mathbb{C}^{p_i}) \otimes \mathbb{1}_{q_i}. \tag{2.4}$$

2.5 Commutant

If $\mathfrak{B} \subset B(\mathcal{H})$, then the *commutant* of $\mathfrak{B}$ is defined as

$$\mathfrak{B}' := \{A \in B(\mathcal{H}) \ : \ AB = BA, \ B \in \mathfrak{B}\}.$$

Theorem 2.2. *1. A commutant is always an algebra containing $\mathbb{1}_{\mathcal{H}}$.*

2. If $\mathfrak{B}$ is $*$-invariant, then so is $\mathfrak{B}'$.

3. $\mathfrak{B}' = \mathfrak{B}''' = \dots$.

4. $\mathfrak{B} \subset \mathfrak{B}'' = \mathfrak{B}'''' = \dots$.

Proof. 1. and 2. are immediate. The following inclusions are easy and they imply 3. and 4.:

$$\mathfrak{B}_1 \subset \mathfrak{B}_2 \quad \Rightarrow \quad \mathfrak{B}_1' \supset \mathfrak{B}_2', \tag{2.5}$$

$$\mathfrak{B} \subset \mathfrak{B}''. \tag{2.6}$$

□

We say that $\mathfrak{A} \subset B(\mathcal{H})$ is a *von Neumann algebra* if $\mathfrak{A} = \mathfrak{A}''$. Clearly, von Neumann algebras are $*$-algebras.

It is easy to see that all $*$-subalgebras of $B(\mathbb{C}^N)$ containing $\mathbb{1}_N$ are von Neumann algebras. Indeed, if $\mathfrak{A}$ is given by (2.4), then $\mathfrak{A}$ is obviously $*$-invariant and

$$\mathfrak{A}' = \bigoplus_{i=1}^{n} \mathbb{1}_{p_i} \otimes B(\mathbb{C}^{q_i}).$$

So, $\mathfrak{A}'' = \mathfrak{A}$.

2.6 Observables – infinite dimension

In infinite dimensions we have several technical complications of the formalism developed in the previous section.

It is still reasonable to assume that observables are described by self-adjoint elements of a $*$-algebra. However, the theory of $*$-algebras is much richer in infinite dimension. Here are a few examples of algebras acting on an infinite dimensional $\mathcal{H}$:

1. Finite rank operators on $\mathcal{H}$.
2. Compact operators on $\mathcal{H}$.
3. Bounded operators on $\mathcal{H}$, that is, $B(\mathcal{H})$.
4. Bounded multiplication operators on $\mathcal{H} = l^2(\mathbb{N})$. This algebra is isomorphic to $l^\infty(\mathbb{N})$.
5. Bounded multiplication operators on $\mathcal{H} = L^2(\mathbb{R})$. This algebra is isomorphic to $L^\infty(\mathbb{R})$.

The definition of a von Neumann algebra is still valid in any dimension. But Theorem 2.1 does not extend to infinite dimension. Besides, there are other kinds of $*$-algebras that are interesting candidates for a description of quantum systems, such as *C^*-algebras*. We will however stick to von Neumann algebras. Note that in the list above only 3,4,5 are von Neumann algebras.

If $\mathfrak{B}$ is a $*$-invariant subset of $B(\mathcal{H})$, then $\mathfrak{B}''$ is the smallest von Neumann algebra containing $\mathfrak{B}$. We will say that $\mathfrak{B}''$ is generated by $\mathfrak{B}$. For instance, the von Neumann algebra generated by finite rank or compact operators is the whole $B(\mathcal{H})$.

Physically, if we know that self-adjoint operators $A_1, \dots, A_n$ are observables, then as the observable algebra it is natural to take

$$\mathfrak{A} = \{A_1, \dots, A_n\}''.$$

Observables are often described by *unbounded self-adjoint operators*. This is not a serious problem. What is relevant for quantum measurements are spectral projections, which are bounded. Thus by saying that an algebra $\mathfrak{A} \subset B(\mathcal{H})$ is generated by $A_1, \dots, A_n$ we will mean that it is generated by spectral projections of these operators (or, equivalently, by their bounded Borel function).

1. Consider the operators $\hat{\phi}_i$, $i = 1, 2, 3$ on $L^2(\mathbb{R}^3)$. They are self-adjoint and commute. They have simple joint spectrum. The von Neumann algebra generated by $\hat{\phi}_i$, $i = 1, 2, 3$ is equal to the operators of multiplication by functions in $L^\infty(\mathbb{R}^3)$.
2. Consider in addition the operators $\hat{\pi}_i := \mathrm{i}^{-1}\partial_{x_i}$, $i = 1, 2, 3$ on $L^2(\mathbb{R}^3)$. The von Neumann algebra generated by $\hat{\phi}_i$, $\hat{\pi}_i$, $i = 1, 2, 3$, coincides with $B(L^2(\mathbb{R}^3))$.

2.7 Haag-Kastler axioms for observable algebras

Let us assume that there are no fermions. Recall that the relativistic covariance of a quantum system described by a Hilbert space $\mathcal{H}$ is expressed by choosing a strongly continuous unitary representation of the connected Poincaré group

$$\mathbb{R}^{1,3} \rtimes SO_0(1,3) \ni (y,\Lambda) \mapsto U(y,\Lambda) \in U(\mathcal{H}), \tag{2.7}$$

which defines the 4-momentum P such that $U(x,\mathbb{1}) = \mathrm{e}^{\mathrm{i}xP}$. We assume the basic requirements of relativistic quantum mechanics, which we recall:

(1) *Existence of a Poincaré invariant vacuum*: There exists a (normalized) vector Ω invariant with respect to $\mathbb{R}^{1,3} \rtimes SO_0(1,3)$.

(2) *Spectral condition*: The joint spectrum of the energy-momentum operator is contained in the forward light cone, that is, $\mathrm{sp}(P) \subset J^+$.

(3) *Uniqueness of the vacuum*: The vector Ω is unique up to a phase factor.

We still need some postulates that express the idea of causality. In the mathematical physics literature one can find two kinds of axioms that try to formalize this concept: the *Haag-Kastler* and the *Wightman axioms*. Even though the Wightman axioms were formulated earlier, it is more natural to start with the Haag-Kastler axioms.

Definition 2.3. *In addition to the basic requirements of relativistic quantum mechanics, suppose to each open bounded set $\mathcal{O} \subset \mathbb{R}^{1,3}$ we associate a* von Neumann algebra $\mathfrak{A}(\mathcal{O}) \subset B(\mathcal{H})$. *We will say that the family $\{\mathfrak{A}(\mathcal{O})\}_{\mathcal{O}}$ is a* net of observable algebras *satisfying the* Haag-Kastler axioms *if the following conditions hold:*

(1) Isotony*: $\mathcal{O}_1 \subset \mathcal{O}_2$ implies $\mathfrak{A}(\mathcal{O}_1) \subset \mathfrak{A}(\mathcal{O}_2)$.*

(2) Poincaré covariance*: for $(y,\Lambda) \in \mathbb{R}^{1,3} \rtimes SO_0(1,3)$, we have*

$$U_{(y,\Lambda)}\mathfrak{A}(\mathcal{O})U^*_{(y,\Lambda)} = \mathfrak{A}\big((y,\Lambda)\mathcal{O}\big).$$

(3) Einstein causality*: Let $\mathcal{O}_1 \times \mathcal{O}_2$. Then*

$$A_i \in \mathfrak{A}(\mathcal{O}_i),\ i = 1,2,\ \textit{implies}\ A_1A_2 = A_2A_1.$$

Self-adjoint elements of the algebras $\mathfrak{A}(\mathcal{O})$ are supposed to describe *observables in $\mathcal{O}$*. This means that in principle an observer contained in $\mathcal{O}$ can measure a self-adjoint operator from $\mathfrak{A}(\mathcal{O})$, and only from $\mathfrak{A}(\mathcal{O})$.

Remark 2.4. *One can ask why von Neumann algebras are used in the Haag-Kastler axioms to describe sets of observables. We would like to argue that it is a natural choice.*

Suppose we weaken the Haag-Kastler axioms as follows: We replace the family of von Neumann algebras $\mathfrak{A}(\mathcal{O})$ by arbitrary sets $\mathfrak{B}(\mathcal{O})$ of self-adjoint elements of $B(\mathcal{H})$, and otherwise we keep the axioms unchanged. Then, if we set $\mathfrak{A}(\mathcal{O}) := \mathfrak{B}(\mathcal{O})''$ (which obviously contain $\mathfrak{B}(\mathcal{O})$), we obtain a family of von

Neumann algebras satisfying the usual Haag-Kastler axioms. In particular, to see that the Einstein causality still holds, we use the following easy fact:

Let $\mathfrak{B}_1$, $\mathfrak{B}_2$, be two $*$-invariant subsets of $B(\mathcal{H})$ such that

$$A_1 \in \mathfrak{B}_1,\ A_2 \in \mathfrak{B}_2 \quad \textit{implies} \quad A_1A_2 = A_2A_1.$$

Set $\mathfrak{A}_1 := \mathfrak{B}_1''$, $\mathfrak{A}_2 := \mathfrak{B}_2''$. Then

$$A_1 \in \mathfrak{A}_1,\ A_2 \in \mathfrak{A}_2 \quad \textit{implies} \quad A_1A_2 = A_2A_1.$$

In fact, $\mathfrak{B}_1 \subset \mathfrak{B}_2' \quad \Rightarrow \quad \mathfrak{B}_1'' \subset \mathfrak{B}_2'''$.

2.8 Quantum fields

In practical computations of quantum field theory the information is encoded in *quantum fields*. In practice, fields are divided into neutral and charged fields, which are described in somewhat different formalisms. However, since charged fields can be decomposed into neutral fields, we will restrict ourselves to neutral fields.

Again, we will restrict ourselves to bosonic fields. They are typically denoted by $\mathbb{R}^{1,3} \ni x \mapsto \hat{\phi}_a(x)$, where $a = 1, \ldots, n$ enumerates the "internal degrees of freedom", eg. the species of particles and the value of their spin projected on a distinguished axis. They commute for spatially separated points, which is expressed by the commutation relations

$$[\hat{\phi}_a(x), \hat{\phi}_b(y)] = 0, \quad (x-y)^2 > 0.$$

One can try to interpret quantum fields as "operator valued tempered distributions", which become (possibly unbounded) self-adjoint operators when smeared out with real Schwartz test functions. We can organize the internal degrees of freedom of neutral fields into a finite dimensional vector space $\mathcal{V} = \mathbb{R}^n$. Thus for any $f = (f_a) \in \mathcal{S}(\mathbb{R}^{1,3}, \mathbb{R}^n)$ we obtain a *smeared-out quantum field*, which is the operator

$$\hat{\phi}[f] := \sum_a \int f_a(x)\hat{\phi}_a(x)\mathrm{d}x. \tag{2.8}$$

2.9 Wightman axioms for bosonic fields

Let us now formulate the Wightman axioms for neutral fields.

Definition 2.5. *We assume that the basic requirements of Relativistic Quantum Mechanics are satisfied and $\mathcal{V}$ is a finite dimensional real vector space equipped with a representation*

$$SO_0(1,3) \ni \Lambda \mapsto \sigma(\Lambda) \in L(\mathcal{V}). \tag{2.9}$$

We suppose that $\mathcal{D}$ is a dense subspace of $\mathcal{H}$ containing Ω and we have a map

$$\mathcal{S}(\mathbb{R}^{1,3}, \mathcal{V}) \ni f \mapsto \hat{\phi}[f] \in L(\mathcal{D}) \tag{2.10}$$

satisfying the following conditions:

(1) Continuity*: For any* $\Phi, \Psi \in \mathcal{D}$*,*

$$\mathcal{S}(\mathbb{R}^{1,3}, \mathcal{V}) \ni f \mapsto (\Phi|\hat{\phi}[f]\Psi) \tag{2.11}$$

is continuous.

(2) Poincaré covariance*: for* $(y, \Lambda) \in \mathbb{R}^{1,3} \rtimes SO_0(1,3)$ *we have*

$$U_{(y,\Lambda)}\hat{\phi}[f]U^*_{(y,\Lambda)} = \hat{\phi}\left[\sigma(\Lambda)f \circ (y,\Lambda)^{-1}\right].$$

(3) Einstein causality*: Let* $\mathrm{supp}f_1 \times \mathrm{supp}f_2$*. Then*

$$\hat{\phi}[f_1]\hat{\phi}[f_2] = \hat{\phi}[f_2]\hat{\phi}[f_1].$$

(4) Cyclicity of the vacuum*: Let* $\mathfrak{F}^{\mathrm{alg}}$ *denote the algebra of polynomials generated by* $\hat{\phi}[f]$*. Then* $\mathfrak{F}^{\mathrm{alg}}\Omega$ *is dense in* $\mathcal{H}$*.*

(5) Hermiticity*: For any* $\Phi, \Psi \in \mathcal{D}$*,*

$$(\Phi|\hat{\phi}[f]\Psi) = (\hat{\phi}[f]\Phi|\Psi).$$

In what follows a map (2.10) satisfying Axiom (1) will be called an *operator valued distribution*. By saying that it is cyclic we will mean that it satisfies Axiom (4).

Note that free bosons satisfy both the Haag-Kastler and Wightman axioms. In particular, the joint spectrum of the Hamiltonian and momentum is contained in the forward light cone:

$$\mathrm{sp}(P) = \{0\} \cup \{p \in \mathbb{R}^{1,3} \mid p^2 = -m^2 \quad \text{or} \quad p^2 \leq -4m^2; \quad p^0 \geq 0\}. \tag{2.12}$$

This follows from the following inequality on the relativistic energy:

$$\sqrt{\vec{p}^2 + m^2} + \sqrt{\vec{k}^2 + m^2} \geq \sqrt{(\vec{p} + \vec{k})^2 + 4m^2}, \tag{2.13}$$

which is saturated for $\vec{p} = \vec{k}$.

It is easy to extend the Haag-Kastler and Wightman axioms to include fermions. The Poincaré group $\mathbb{R}^{1,3} \rtimes SO_0(1,3)$ has to be replaced by its 2-fold covering $\mathbb{R}^{1,3} \rtimes Spin_0(1,3)$, and (in the case of Wightman axioms) we should allow for anticommutation between fields.

2.10 Relationship between Haag-Kastler and Wightman axioms

"Morally", Wightman axioms are stronger than the Haag-Kastler axioms. In fact, let $\mathfrak{A}^{\mathrm{alg}}(\mathcal{O})$ be the algebra of polynomials in $\hat{\phi}[f]$ with $\mathrm{supp}f \subset \mathcal{O}$, which can be treated as a $*$-subalgebra of $L(\mathcal{D})$. Then the family $\mathcal{O} \mapsto \mathfrak{A}^{\mathrm{alg}}(\mathcal{O})$ is almost a net of field algebras. Unfortunately, elements of $\mathfrak{A}^{\mathrm{alg}}(\mathcal{O})$ are defined

only on $\mathcal{D}$ and not on the whole $\mathcal{H}$, and often do not extend to bounded operators on $\mathcal{H}$.

We know that the fields $\hat{\phi}[f]$ are *Hermitian* (symmetric) on $\mathcal{D}$. Suppose they are *essentially self-adjoint*. Then their closures are self-adjoint operators on $\mathcal{H}$. We could consider the von Neumann algebra $\mathfrak{A}(\mathcal{O})$ generated by bounded functions of $\hat{\phi}[f]$, $\mathrm{supp} f \subset \mathcal{O}$. Then there is still no guarantee that the net $\mathcal{O} \mapsto \mathfrak{A}_0(\mathcal{O})$ satisfies the Haag-Kastler axioms: we are not sure whether the Einstein causality holds.

To understand this, we recall that there are serious problems with commutation of unbounded operators [Reed-Simon-I]. One says that two self-adjoint operators commute (or strongly commute) if all their spectral projections commute. There exist however examples of pairs of two self-adjoint operators A, B and a subspace $\mathcal{D} \subset \mathrm{Dom}A \cap \mathrm{Dom}B$ with the following property:

(1) A and B preserve $\mathcal{D}$ and are essentially self-adjoint on $\mathcal{D}$.

(2) A and B commute on $\mathcal{D}$.

(3) A and B do not commute strongly.

(4) $\mathcal{D}$ is dense.

One of the most important topics in QFT is that of gauge invariance. In the older literature one distinguishes between gauge invariance of the first kind–wrt a global symmetry–and of the second kind–wrt a local symmetry. In modern physics literature the first meaning seems to have disappeared, although it is still used in some parts of mathematical literature. Thus in the modern physics usage by gauge invariance one one means *local* gauge invariance.

Global symmetries are well understood in the framework of Haag-Kastler axioms, thanks to the work of Doplicher-Haag-Roberts. Unfortunately, to my understanding, we do not know how to accommodate (local) gauge invariance in axioms of QFT.

The Haag-Kastler axioms are so abstract, general and have so little structure that we do not know how to see the gauge invariance. The Wightman axioms do not apply to gauge fields, because apparently for them one needs an indefinite product Hilbert space or nonlocal fields like Wilson loops. I am not aware of a successful adaptation of Wightman axioms that accommodates gauge fields.

3 The Laplace and Helmholtz equation

3.1 Tempered distributions

The space of *Schwartz functions on* $\mathbb{R}^n$ is defined as

$$\mathcal{S}(\mathbb{R}^n) := \big\{ \Psi \in C^\infty(\mathbb{R}^n) \ : \ \int |x^\alpha \nabla_x^\beta \Psi(x)|^2 \mathrm{d}x < \infty, \quad \alpha, \beta \in \mathbb{N}^n \big\}. \tag{3.1}$$

Remark 3.1. *(3.1) is equivalent to the definition*

$$\mathcal{S}(\mathbb{R}^n) = \big\{ \Psi \in C^\infty(\mathbb{R}^n) \ : \ |x^\alpha \nabla_x^\beta \Psi(x)| \leq c_{\alpha,\beta}, \quad \alpha, \beta \in \mathbb{N}^n \big\}. \tag{3.2}$$

more common in the literature.

$\mathcal{S}'(\mathbb{R}^n)$ denotes the space of continuous linear functionals on $\mathcal{S}(\mathbb{R}^n)$. This means. a linear functional $\mathcal{S}(\mathbb{R}^n) \ni \Psi \mapsto \langle T|\Psi\rangle \in \mathbb{C}$ belongs to $\mathcal{S}'$ iff there exists N such that

$$|\langle T|\Psi\rangle| \leq C\Big(\sum_{|\alpha|+|\beta|<N} \int |x^\alpha \nabla_x^\beta \Psi(x)|^2 \mathrm{d}x\Big)^{\frac{1}{2}}.$$

If f is a function which is locally integrable (L^1 on all bounded intervals), and satisfies some mild growth conditions, then it defines a distribution in $\mathcal{S}'$ by the formula

$$\langle T_f|\Psi\rangle = \int f(x)\Psi(x)\mathrm{d}x. \tag{3.3}$$

Motivated by (3.3), we will often use the integral notation

$$\langle T|\Psi\rangle = \int T(x)\Psi(x)\mathrm{d}x$$

also for distributions that are not given by such integrals

Here are some examples of elements of $\mathcal{S}'(\mathbb{R})$:

$$\int \delta(t)\Phi(t)\mathrm{d}t := \Phi(0), \tag{3.4}$$

$$\mathcal{P}\int \frac{\Phi(x)}{x}\mathrm{d}x := \lim_{\epsilon\searrow 0}\left(\int_{-\infty}^{\epsilon} + \int_{\epsilon}^{+\infty}\right)\frac{\Phi(x)}{x}\mathrm{d}x, \tag{3.5}$$

$$\int (t \pm \mathrm{i}0)^\lambda \Phi(t)\mathrm{d}t := \lim_{\epsilon\searrow 0}\int (t \pm \mathrm{i}\epsilon)^\lambda \Phi(t)\mathrm{d}t. \tag{3.6}$$

(3.6) is simply given by the locally integrable function t^λ, however for $\lambda < -1$ it is not.

Here some examples of functions that do not correspond to elements of $\mathcal{S}'(\mathbb{R})$: e^t, $\frac{1}{|t|}$, $\frac{1}{t}$. The first blows up at infinity too fast. The last two can be regularized to make a distribution in $\mathcal{S}'(\mathbb{R})$. Note the *Sochocki formula* and its consequence:

$$\frac{1}{t \mp \mathrm{i}0} = \mathcal{P}\frac{1}{t} \pm \mathrm{i}\pi\delta(t), \tag{3.7}$$

$$\frac{1}{t-\mathrm{i}0} - \frac{1}{t+\mathrm{i}0} = 2\pi\mathrm{i}\delta(t). \tag{3.8}$$

Note that for $\lambda > -1$

3.2 Fourier transformation

The definition of the Fourier transform of $\mathbb{R}^d \ni \vec{x} \mapsto f(\vec{x})$ on a Euclidean space will be standard:

$$\hat{f}(\vec{k}) := \int \mathrm{e}^{-\mathrm{i}\vec{k}\cdot\vec{x}} f(\vec{x})\mathrm{d}\vec{x}.$$

It is also common normalize the Fourier transformation as follows

$$\mathcal{F}f(k) = \frac{1}{\sqrt{(2\pi)^d}}\hat{f}(k).$$

$\mathcal{F}$ is unitary on $L^2(\mathbb{R}^d)$.

Often, we will drop the hat – the name of the variable will indicate whether we use the position or momentum representation:

$$f(\vec{k}) = \int \mathrm{e}^{-\mathrm{i}\vec{k}\cdot\vec{x}} f(\vec{x})\mathrm{d}\vec{x}, \quad f(\vec{x}) = \frac{1}{(2\pi)^d}\int \mathrm{e}^{\mathrm{i}\vec{k}\cdot\vec{x}} f(\vec{k})\mathrm{d}\vec{k}.$$

On a Minkowski space, for the time variable (typically t) we reverse the sign in the Fourier transform:

$$f(\varepsilon) = \int \mathrm{e}^{\mathrm{i}\varepsilon t} f(t)\mathrm{d}t, \quad f(t) = \frac{1}{2\pi}\int \mathrm{e}^{-\mathrm{i}\varepsilon t} f(\varepsilon)\mathrm{d}\varepsilon.$$

The Fourier transformation is a continuous map from $\mathcal{S}'$ into itself. We have continuous inclusions

$$\mathcal{S}(\mathbb{R}^n) \subset L^2(\mathbb{R}^n) \subset \mathcal{S}'(\mathbb{R}^n).$$

3.3 Green's functions on the Euclidean space

Let $\mathbb{R}^d$ be the Euclidean space and Δ the Laplacian. The following equations are invariant wrt $\mathbb{R}^d \rtimes O(d)$:

$$\text{the } \textit{Laplace equation} \qquad -\Delta\zeta = 0, \tag{3.9}$$

$$\text{the } \textit{Helmholtz equation} \qquad (-\Delta \pm m^2)\zeta = 0. \tag{3.10}$$

We also have their inhomogeneous versions:

$$\text{the } \textit{Poisson equation} \qquad -\Delta\zeta = f, \tag{3.11}$$

$$\text{the } \textit{inhomogeneous Helmholtz equation} \qquad (-\Delta \pm m^2)\zeta = f. \tag{3.12}$$

We will say that G is *Green's function* for $-\Delta \pm m^2$ if

$$(-\Delta \pm m^2)G(x) = \delta(x). \tag{3.13}$$

If we are given f and G is Green's function, then

$$\zeta(x) = \int G(x-y)f(y)\mathrm{d}y \tag{3.14}$$

solves (3.12)

Assume that $\zeta, f \in \mathcal{S}'(\mathbb{R}^d)$ and apply the Fourier transformation

$$\zeta(x) = (2\pi)^{-d}\int \mathrm{e}^{\mathrm{i}px}\zeta(p)\mathrm{d}p, \quad f(x) = (2\pi)^{-d}\int \mathrm{e}^{\mathrm{i}px} f(p)\mathrm{d}p \tag{3.15}$$

to (3.12). Then

$$(p^2+m^2)\zeta(p)=f(p),\quad \zeta(p)=(p^2+m^2)^{-1}f(p) \tag{3.16}$$

Using $\widehat{G\star f}=\hat{G}\hat{f}$ we obtain

$$\zeta(x)=\int G_{d,m}(x-y)f(y)\mathrm{d}y,\quad G_{d,m}(x)=(2\pi)^{-d}\int\frac{\mathrm{e}^{\mathrm{i}xp}}{(p^2+m^2)}\mathrm{d}p. \tag{3.17}$$

For $m>0$ or $m=0$ and $d\neq 1,2$, the function $(p^2+m^2)^{-1}$ is locally integrable and belongs to $\mathcal{S}'(\mathbb{R}^d)$. Hence its Fourier transform is well defined and is the unique Green's function of $-\Delta+m^2$ (at least if we are interested only in solutions in $\mathcal{S}'(\mathbb{R}^d)$, which is usually the case).

The case $m>0$ can be reduced to $m=1$:

$$G_{d,m}(x)=m^{d-2}G_d(mx),\quad G_d(x)=(2\pi)^{-d}\int\frac{\mathrm{e}^{\mathrm{i}xp}}{(p^2+1)}\mathrm{d}p. \tag{3.18}$$

The Euclidean invariance suggests to look for Green's functions that depend only on $r=|x|$, so that one can write $G(x)=G(r)$. Such Green's functions away from $r=0$ satisfy the radial part of the Helmholtz equation:

$$\Big(-\partial_r^2-\frac{d-1}{r}\partial_r\pm m^2\Big)G(r)=0 \tag{3.19}$$

The massless Green's function can be expressed in terms of elementary functions.

Theorem 3.2. *For $d\geq 3$, $G_{d,0}(r)=\frac{\Gamma(\frac{d}{2}-1)}{4\pi^{\frac{d}{2}}}r^{2-d}$.*
E.g. $G_{3,0}(r)=\frac{1}{4\pi r}$, $G_{4,0}(r)=\frac{1}{4\pi^2r^2}$.

Proof. It is elementary to check that $G(r)=c_dr^{2-d}$ satisfies the Laplace equation away from the origin. Clearly, it belongs to $\mathcal{S}'(\mathbb{R}^d)$. We need to find c_d. We take a radial test function $\Psi(r)$. We need to check that

$$-\Delta G_{d,0}(x)=\delta(x), \tag{3.20}$$

$$\text{or}\quad \int\Delta G(x)\Phi(x)\mathrm{d}x=-\Phi(0). \tag{3.21}$$

But the lhs of (3.21) equals

$$\int G(x)\Delta\Phi(x)\mathrm{d}x=\int_0^\infty G(r)r^{d-1}|\mathbb{S}_{d-1}|\Big(\partial_r^2+\frac{d-1}{r}\partial_r\Big)\Phi(r)\mathrm{d}r \tag{3.22}$$

$$=c_d|\mathbb{S}_{d-1}|\bigg(\int_0^\infty\Phi(r)\Big(\partial_r^2-\partial_r\frac{d-1}{r}\Big)r\mathrm{d}r \tag{3.23}$$

$$+\big(r\Phi'(0)-\Phi(0)+(d-1)\Phi(0)\big)\bigg)\Big|_0^\infty \tag{3.24}$$

$$=c_d|\mathbb{S}_{d-1}|(d-2)\Phi(0), \tag{3.25}$$

where $|\mathbb{S}_{d-1}| = \frac{2\pi^d}{\Gamma(\frac{d}{2})}$ is the surface of the $d-1$-dimensional sphere.

In the massive case, For $d \geq 3$, $G_{d,m}(r) \sim \frac{\Gamma(\frac{d}{2}-1)}{4\pi^{\frac{d}{2}}} r^{2-d}$. near zero, but for large r we have exponential decay, more precisely

$$G_{d,m}(r) \sim \frac{1}{2(2\pi)^{\frac{d-1}{2}}} r^{\frac{1-d}{2}} \mathrm{e}^{-mr}. \tag{3.26}$$

This will follow from the analysis below.

3.4 Bessel equations

There are two basic forms of the *Bessel equation*:

$$\text{the } \textit{modified Bessel equation} \qquad \Big(\partial_r^2 + \frac{1}{r}\partial_r - \frac{\mu^2}{r^2} - 1\Big)v = 0, \tag{3.27}$$

$$\text{the } \textit{(standard) Bessel equation} \qquad \Big(\partial_r^2 + \frac{1}{r}\partial_r - \frac{\mu^2}{r^2} + 1\Big)v = 0. \tag{3.28}$$

One can pass from one to the other by substituting $\pm \mathrm{i}r$ for r.

We have

$$r^{-1+\frac{d}{2}}\Big(\partial_r^2 + \frac{d-1}{r}\partial_r\Big)r^{-\frac{d}{2}+1} = \partial_r^2 + \frac{1}{r}\partial_r - \Big(1-\frac{d}{2}\Big)^2\frac{1}{r^2}, \tag{3.29}$$

Set $\mu = \frac{d}{2} - 1$ and $m = 1$. We see that if F satisfies satisfies the modified Bessel equation, then $r^{1-\frac{d}{2}}F(r)$ satisfies (3.19) for $+m^2$, and if F satisfies the standard Bessel equation is, then $r^{1-\frac{d}{2}}F(r)$ satisfies (3.19) for $-m^2$.

3.5 Macdonald function

One of standard solutions of the modified Bessel equation is the *Macdonald function:*

$$K_\mu(r) \quad := \quad \frac{1}{2}\int_0^\infty \exp\Big(-\frac{r}{2}(s+s^{-1})\Big)\, s^{\pm\mu-1}\mathrm{d}s. \tag{3.30}$$

The integral (3.30) is absolutely convergent. Substitution $s = t^{-1}$ shows that μ can be replaced by $-\mu$ (and thus $K_\mu = K_{-\mu}$).

Theorem 3.3. *For* $|\arg z| < \pi - \epsilon$,

$$\lim_{|z|\to\infty} \frac{K_\mu(z)}{\frac{\mathrm{e}^{-z}\sqrt{\pi}}{\sqrt{2z}}} = 1.$$

Proof. We use the *steepest descent method.* Set $\phi(t) := -\frac{1}{2}(t + t^{-1})$. We compute

$$\phi'(t) = -\frac{1}{2}(1-t^{-2}), \quad \phi''(t) = -t^{-3}.$$

Hence ϕ has a critical point at $t_0 = 1$ with $\phi(t_0) = -1$ and $\phi''(t_0) = -1$. Thus

$$\begin{aligned} K_\mu(z) &= \frac{1}{2}\int_0^\infty t^{-\mu-1}\exp(z\phi(t))\mathrm{d}t \\ &\simeq \frac{1}{2}\int_{-\infty}^\infty \exp\left(z\phi(t_0) + z\frac{\phi''(t_0)}{2}(t-t_0)^2\right)\mathrm{d}t \\ &= \frac{1}{2}\mathrm{e}^{-z}\int_{-\infty}^\infty \exp\left(\frac{z}{2}(t-1)^2\right)\mathrm{d}t \;=\; \frac{1}{2}\mathrm{e}^{-z}\frac{\sqrt{2\pi}}{\sqrt{z}}. \end{aligned}$$

□

Theorem 3.4. *For $\mu > 0$,*

$$\lim_{m\searrow 0} m^\mu K_\mu(mr) = \frac{1}{2}\Gamma(\mu)\Big(\frac{r}{2}\Big)^{-\mu}. \tag{3.31}$$

Proof. We set $s = \frac{2t}{mr}$:

$$m^\mu K_\mu(mr) = \frac{m^\mu}{2}\int_0^\infty \exp\left(-\frac{mr}{2}(s+s^{-1})\right)s^{\mu-1}\mathrm{d}s \tag{3.32}$$

$$= \frac{1}{2}\Big(\frac{2}{r}\Big)^\mu \int_0^\infty \exp\left(-t - \frac{m^2r^2}{4t}\right)t^{\mu-1}\mathrm{d}t \tag{3.33}$$

$$\to \frac{1}{2}\Big(\frac{r}{2}\Big)^{-\mu}\Gamma(\mu). \tag{3.34}$$

□

For half-integer μ the Macdonald function can be expressed in terms of elementary functions, e.g.

$$K_{\pm\frac{1}{2}}(r) = \Big(\frac{\pi}{2r}\Big)^{\frac{1}{2}}\mathrm{e}^{-r}. \tag{3.35}$$

Theorem 3.5.

$$G_d(r) = \frac{1}{(2\pi)^{\frac{d}{2}}}r^{1-\frac{d}{2}}K_{\frac{d}{2}-1}(r). \tag{3.36}$$

E.g. $G_1(r) = \frac{\mathrm{e}^{-r}}{2}$, $G_3(r) = \frac{\mathrm{e}^{-r}}{4\pi r}$.

Proof. We will use the following identities:

$$\frac{1}{A} = \int_0^\infty \mathrm{e}^{-sA}\mathrm{d}s, \tag{3.37}$$

$$\int \mathrm{d}p\mathrm{e}^{-\frac{sp^2}{2}}\mathrm{e}^{\mathrm{i}px} = \Big(\frac{2\pi}{s}\Big)^{\frac{d}{2}}\mathrm{e}^{-\frac{x^2}{2s}}. \tag{3.38}$$

Now

$$\begin{aligned}
& (2\pi)^{-d}\int \frac{\mathrm{e}^{\mathrm{i}px}\mathrm{d}p}{(1+p^2)} \\
= \;& (2\pi)^{-d}\frac{|x|}{2}\int_0^\infty \mathrm{d}s\int \mathrm{d}p \mathrm{e}^{-(1+p^2)\frac{|x|s}{2}}\mathrm{e}^{\mathrm{i}px} \\
= \;& (2\pi)^{-d}\Big(\frac{|x|}{2}\Big)^{1-\frac{d}{2}}\pi^{\frac{d}{2}}\int_0^\infty \mathrm{d}s s^{-\frac{d}{2}}\mathrm{e}^{-(s+\frac{1}{s})\frac{|x|}{2}} \\
= \;& (2\pi)^{-d}2\pi^{\frac{d}{2}}\Big(\frac{|x|}{2}\Big)^{1-\frac{d}{2}}K_{1-\frac{d}{2}}(|x|).
\end{aligned}$$

□

Using

$$G_{d,0}(x) = \lim_{m\searrow 0} m^{d-2}G_d(mx), \tag{3.39}$$

we obtain an alternative proof of the zero mass formulas $G_{d,0}(r) = \frac{\Gamma(\frac{d}{2}-1)}{4\pi^{\frac{d}{2}}}r^{2-d}$, $d \geq 3$.

3.6 Bessel and Hankel functions

We will also need the following solutions of the standard Bessel equation:

$$\text{the } \textit{Hankel functions}\text{:} \quad H_\mu^{(1)/(2)}(r) = H_\mu^{\pm}(r) := \frac{2}{\pi}\mathrm{e}^{\mp \mathrm{i}\frac{\pi}{2}(\mu+1)}K_\mu(\mp \mathrm{i}r), \tag{3.40}$$

$$\text{the } \textit{Bessel function}\text{:} \quad J_\mu(r) := \frac{1}{2}\big(H_\mu^+(r) + H_\mu^-(r)\big) \tag{3.41}$$

For large $r > 0$ the Hankel functions are oscillating:

$$\lim_{r\to\infty}\frac{H_\mu^{\pm}(r)}{\big(\frac{2}{\pi r}\big)^{\frac{1}{2}}\mathrm{e}^{\pm \mathrm{i}r}\mathrm{e}^{\mp\frac{\mathrm{i}\mu\pi}{2}\mp\frac{\mathrm{i}\pi}{4}}} = 1,$$

The Bessel function can be expanded in a power series near zero:

$$J_\mu(r) \;\; = \;\; \sum_{n=0}^\infty \frac{(-1)^n\left(\frac{r}{2}\right)^{2n+\mu}}{n!\Gamma(\mu+n+1)}.$$

Let's go back to the Helmholtz equation with the negative sign at m^2:

$$(-\Delta - m^2)\zeta = f. \tag{3.42}$$

The Green's function $G_{d,m}$ is well defined not only for $m \geq 0$, but also for $\mathrm{Re}(m) > 0$, which guarantees $m^2 \in \mathbb{C}\backslash]-\infty, 0]$. Taking the limit at imaginary line, that is setting $G_{d,\pm \mathrm{i}m}$, we obtain two Green's functions of (3.42):

$$G_{d,\mp \mathrm{i}m}(r) = (2\pi)^{-d}\int \frac{\mathrm{e}^{-\mathrm{i}xp}}{(p^2 - m^2 \mp \mathrm{i}0)}\mathrm{d}p \tag{3.43}$$

$$= \pm\frac{\mathrm{i}}{4}\Big(\frac{m}{2\pi r}\Big)^{\frac{d}{2}-1}H^{\pm}_{\frac{d}{2}-1}(mr). \tag{3.44}$$

Thus in the case $-m^2$ we have many Green's functions that belong to $\mathcal{S}'$. We also have many solutions in $\mathcal{S}'$ of the (homogeneous) Helmholtz equation, e.g.

$$\mathrm{i}\big(G_{d,\mathrm{i}m}(r) - G_{d,-\mathrm{i}m}(r)\big) = \frac{1}{2}\Big(\frac{m}{2\pi r}\Big)^{\frac{d}{2}-1} J_{\frac{d}{2}-1}(mr). \tag{3.45}$$

4 Wave and Klein-Gordon equations

4.1 Propagators

Let $d = 1 + n$. Let $\Box$ be the d'Alembertian on the Minkowski space $\mathbb{R}^{1,n}$:

$$\Box := -\partial_0^2 + \sum_{i=1}^{n} \partial_i^2. \tag{4.1}$$

The following equations are invariant wrt $\mathbb{R}^{1+n} \rtimes O(1,n)$:

$$\text{the } \textit{wave equation} \qquad -\Box\zeta = 0, \tag{4.2}$$

$$\text{the } \textit{Klein-Gordon equation} \qquad (-\Box + m^2)\zeta = 0. \tag{4.3}$$

We are interested also in their inhomogeneous versions:

$$\text{the } \textit{inhomogeneous wave equation} \qquad -\Box\zeta = f, \tag{4.4}$$

$$\text{the } \textit{inhomogeneous Klein-Gordon equation} \qquad (-\Box + m^2)\zeta = f. \tag{4.5}$$

We will say that $G^\bullet$ is Green's function of the Klein-Gordon equation if

$$(-\Box + m^2)G^\bullet(x) = \delta(x). \tag{4.6}$$

Thus, for any f,

$$\zeta(x) = \int G^\bullet(x-y) f(y) \mathrm{d}y \tag{4.7}$$

satisfies (4.5).

We say that $G^\bullet$ is a solution the Klein-Gordon equation if

$$(-\Box + m^2)G^\bullet(x) = 0. \tag{4.8}$$

The ansatz analogous to (3.17)

$$G^\bullet(x) = (2\pi)^{-d} \int \frac{\mathrm{e}^{\mathrm{i}xp}}{(p^2 + m^2)} \mathrm{d}p \tag{4.9}$$

is incomplete and needs to be precised to make it well defined.

Every bisolution of $G^\bullet$ can be written as

$$G^\bullet(x) \quad = \quad \int \mathrm{e}^{\mathrm{i}px} g(p) \delta(p^2 + m^2) \frac{\mathrm{d}p}{(2\pi)^3}$$

where g is a function on the two-sheeted hyperboloid $p^2 + m^2 = 0$ (see below for the meaning of $\delta(p^2 + m^2)$).

4.2 Invariant measure

Let f be a differentiable function on $\mathbb{R}$. The following fact (under appropriate assumptions) is easy:

Lemma 4.1. *Let δ_ϵ be an approximate delta function, that is*

$$\lim_{\epsilon \searrow 0} \int \delta_\epsilon(t)\phi(t)\mathrm{d}t = \phi(0).$$

Then

$$\int \lim_{\epsilon \searrow 0} \delta_\epsilon(f(s))\phi(s)\mathrm{d}s = \sum_{f(s_i)=0} \frac{\phi(s_i)}{|f'(s_i)|}. \tag{4.10}$$

This suggests the following notation:

$$\int \delta(f(s))\phi(s)\mathrm{d}s = \sum_{f(s_i)=0} \frac{\phi(s_i)}{|f'(s_i)|}. \tag{4.11}$$

Now consider $\mathbb{R}^{1,n}$ and apply (4.11) to $s = p^0$ for fixed $\vec{p}$ and

$$f(p) = p^2 + m^2 = -(p^0)^2 + \vec{p}^2 + m^2.$$

We have

$$\frac{\mathrm{d}(p^2+m^2)}{\mathrm{d}p^0} = 2p^0,$$

and $p^2 + m^2 = 0$ iff $p^0 = \pm\sqrt{\vec{p}^2 + m^2}$. Hence we can write

$$\delta(p^2+m^2)\mathrm{d}p = \frac{\delta\Big(p^0 - \sqrt{\vec{p}^2+m^2}\Big)}{2\sqrt{\vec{p}^2+m^2}}\mathrm{d}\vec{p} + \frac{\delta\Big(p^0 + \sqrt{\vec{p}^2+m^2}\Big)}{2\sqrt{\vec{p}^2+m^2}}\mathrm{d}\vec{p}. \tag{4.12}$$

(4.12) is a measure on $\mathbb{R}^{1,3}$ invariant wrt Lorentz transformations. In fact,

$$2\pi\mathrm{i}\delta(p^2+m^2) = \lim_{\epsilon \searrow 0}\Big(\frac{1}{p^2+m^2-\mathrm{i}\epsilon} - \frac{1}{p^2+m^2+\mathrm{i}\epsilon}\Big), \tag{4.13}$$

where the rhs is obviously Lorentz invariant.

4.3 Propagators for the Klein-Gordon and wave equation

Introduce

- *the forward/backward or retarded/advanced propagator*

$$G^{\vee/\wedge}(x) := \frac{1}{(2\pi)^d}\int \frac{\mathrm{e}^{\mathrm{i}x\cdot p}}{p^2+m^2 \mp \mathrm{i}0\mathrm{sgn}(p^0)}\mathrm{d}p, \tag{4.14a}$$

- the *Feynman/anti-Feynman(-Stueckelberg) propagator*

$$G^{\mathrm{F}/\overline{\mathrm{F}}}(x) := \frac{1}{(2\pi)^d}\int \frac{\mathrm{e}^{\mathrm{i}x\cdot p}}{p^2+m^2\mp \mathrm{i}0}\mathrm{d}p, \tag{4.14b}$$

- the *Pauli–Jordan propagator or the commutator function*

$$G^{\mathrm{PJ}}(x) := \frac{\mathrm{i}}{(2\pi)^d}\int \mathrm{e}^{\mathrm{i}x\cdot p}\mathrm{sgn}(p_0)\delta(p^2+m^2)\mathrm{d}p \tag{4.14c}$$

$$= \frac{1}{(2\pi)^{d-1}}\int \frac{\mathrm{d}\vec{p}}{\sqrt{\vec{p}^2+m^2}}\mathrm{e}^{\mathrm{i}\vec{x}\vec{p}}\sin\left(x^0\sqrt{\vec{p}^2+m^2}\right) \tag{4.14d}$$

- *the positive/negative frequency, or particle/antiparticle, or Wightman-anti-Wightman solution (two-point function)*

$$G^{(\pm)}(x) := \frac{1}{(2\pi)^d}\int \mathrm{e}^{\mathrm{i}x\cdot p}\theta(\pm p_0)\delta(p^2+m^2)\mathrm{d}p \tag{4.14e}$$

$$= \frac{1}{(2\pi)^{d-1}}\int \frac{\mathrm{d}\vec{p}}{2\sqrt{\vec{p}^2+m^2}}\mathrm{e}^{\mp\mathrm{i}x^0\sqrt{\vec{p}^2+m^2}+\mathrm{i}\vec{x}\vec{p}}. \tag{4.14f}$$

(4.14a), (4.14b) are distinguished Green's functions (inverses) and (4.14c), (4.14e) are distinguished solutions of the Klein–Gordon equation $-\Box+m^2$. We will call them jointly "propagators".

Note the identities satisfied by the propagators:

$$G^\vee - G^\wedge = G^{\mathrm{PJ}} \tag{4.15a}$$

$$= \mathrm{i}G^{(+)} - \mathrm{i}G^{(-)}, \tag{4.15b}$$

$$G^{\mathrm{F}} - G^{\overline{\mathrm{F}}} = \mathrm{i}G^{(+)} + \mathrm{i}G^{(-)}, \tag{4.15c}$$

$$G^{\mathrm{F}} + G^{\overline{\mathrm{F}}} = G^\vee + G^\wedge, \tag{4.15d}$$

$$G^{\mathrm{F}} = \mathrm{i}G^{(+)} + G^\wedge = \mathrm{i}G^{(-)} + G^\vee, \tag{4.15e}$$

$$G^{\overline{\mathrm{F}}} = -\mathrm{i}G^{(+)} + G^\vee = -\mathrm{i}G^{(-)} + G^\wedge. \tag{4.15f}$$

To prove these identities we use repeatedly

$$\theta(\pm p^0)2\pi\mathrm{i}\delta(p^2+m^2) = \theta(\pm p^0)\Big(\frac{1}{p^2+m^2-\mathrm{i}0} - \frac{1}{p^2+m^2+\mathrm{i}0}\Big), \tag{4.16}$$

4.4 Einstein causality of propagators

Proposition 4.2. *We have* $\mathrm{supp}G^{\vee/\wedge}\subset J^{\vee/\wedge}$ *and* $\mathrm{supp}G^{\mathrm{PJ}}\subset J$.

Proof. Let us prove that $\mathrm{supp}G^\vee \subset J^\vee$. By the Lorentz invariance it suffices to prove that $G^\vee$ is zero on the lower half-plane. We write

$$\begin{aligned} G^\vee(x) &= \int \frac{\mathrm{e}^{\mathrm{i}px}}{(p^2+m^2-\mathrm{i}0\mathrm{sgn}p^0)}\frac{\mathrm{d}p}{(2\pi)^4} \\ &= \int \frac{\mathrm{e}^{-\mathrm{i}p^0x^0+\mathrm{i}\vec{p}\vec{x}}}{\big(\vec{p}^2+m^2-(p^0+\mathrm{i}0)^2\big)}\frac{\mathrm{d}p^0\mathrm{d}\vec{p}}{(2\pi)^4}. \end{aligned}$$

Next we continuously deform the contour of integration, replacing p^0 by $p^0+\mathrm{i}R$, where $R\in[0,\infty[$. We do not cross any singularities of the integrand and note that $\mathrm{e}^{-\mathrm{i}x^0(p^0+\mathrm{i}R)}$ goes to zero (remember that $x^0<0$).

Analogously one proves $\mathrm{supp}G^\wedge\subset J^\wedge$. By (4.15a) we obtain $\mathrm{supp}G^{\mathrm{PJ}}\subset J$. □

Note that

$$G^{(+)}(x)=\begin{cases}-\mathrm{i}G^{\mathrm{F}}(x) & \text{on } \mathbb{R}^{1,3}\backslash J^\wedge,\\ \mathrm{i}G^{\overline{\mathrm{F}}}(x) & \text{on } \mathbb{R}^{1,3}\backslash J^\vee;\end{cases} \tag{4.17}$$

$$\overline{G^{(+)}(x)}=G^{(-)}(x)=\begin{cases}-\mathrm{i}G^{\mathrm{F}}(x) & \text{on } \mathbb{R}^{1,3}\backslash J^\vee,\\ \mathrm{i}G^{\overline{\mathrm{F}}}(x) & \text{on } \mathbb{R}^{1,3}\backslash J^\wedge.\end{cases} \tag{4.18}$$

Hence

$$-\mathrm{i}G^{\mathrm{F}}(x-y)=\theta(x^0-y^0)G^{(+)}(x-y)+\theta(y^0-x^0)G^{(-)}(x-y), \tag{4.19}$$

$$\mathrm{i}G^{\mathrm{F}}(x-y)=\theta(x^0-y^0)G^{(-)}(x-y)+\theta(y^0-x^0)G^{(+)}(x-y). \tag{4.20}$$

4.5 Propagators in position representation in dimension $1+3$.

Below we give the formulas for the massive propagators in the position representation in dimension $1+3$.

- The forward/backward or retarded/advanced propagator:

$$G^{\vee/\wedge}(x) = \frac{1}{2\pi}\theta(\pm x^0)\delta(x^2)-\frac{m\theta(-x^2)\theta(\pm x^0)}{4\pi\sqrt{-x^2}}J_1(m\sqrt{-x^2}).$$

- The (anti-)Feynman(-Stueckelberg) Green's function:

$$\begin{aligned}G^{\mathrm{F}/\overline{\mathrm{F}}}(x) &= \frac{1}{4\pi}\delta(x^2)-\frac{m\theta(-x^2)}{8\pi\sqrt{-x^2}}H_1^{\mp}(m\sqrt{-x^2})\\ &\quad \pm\frac{mi\theta(x^2)}{4\pi^2\sqrt{x^2}}K_1(m\sqrt{x^2}).\end{aligned} \tag{4.21}$$

- The Pauli-Jordan

$$G^{\mathrm{PJ}}(x) = \frac{1}{2\pi}\mathrm{sgn}x^0\delta(x^2)-\frac{m\mathrm{sgn}x^0\theta(-x^2)}{4\pi\sqrt{-x^2}}J_1(m\sqrt{-x^2}).$$

- The *positive/negative frequency solution*:

$$\begin{aligned}G^{(\pm)}(x) &= \mp\frac{\mathrm{i}}{4\pi}\mathrm{sgn}x^0\delta(x^2)\\ &\quad -\frac{\mathrm{i}m\theta(-x^2)}{8\pi\sqrt{-x^2}}H_1^{\mp\mathrm{sgn}x^0}(m\sqrt{-x^2})+\frac{m\theta(x^2)}{4\pi^2\sqrt{x^2}}K_1(m\sqrt{x^2}).\end{aligned}$$

The above formulas are somewhat sloppily written in the neighborhood of the surface of the light cone, where they describe irregular distribution.

To obtain these formulas, first we find the Euclidean Green's function in 4 dimensions:

$$G^{\mathrm{E}}(x) = \frac{m}{4\pi^2|x|} K_1(m|x|). \tag{4.22}$$

Using the formula for the function K_1 we can write

$$\begin{aligned} G^{\mathrm{E}}(x) &= \frac{1}{4\pi^2|x|^2} + \frac{m^2}{8\pi^2} \sum_{k=0}^{\infty} \Big(\ln \frac{|x|m}{2} + \gamma + \frac{H_k + H_{k+1}}{2} \Big) \frac{1}{k!(k+1)!} \Big(\frac{m^2|x|^2}{4} \Big)^k \\ &= \frac{1}{4\pi^2|x|^2} + m^2 \ln \frac{|x|m}{2} u(m^2|x|^2) + m^2 v(m^2|x|^2), \end{aligned} \tag{4.23}$$

where u, v are analytic functions and $H_k = \frac{1}{1} + \cdots + \frac{1}{k}$. Then we apply the Wick rotation. This means that we replace x^4 with $\pm \mathrm{i} x^0$ in the argument. We also have to replace the measure of integration $\mathrm{d}x^1 \cdots \mathrm{d}x^4$ with $\pm \mathrm{i} \mathrm{d}x^0 \mathrm{d}x^1 \cdots$. This leads to the Feynman/anti-Feynman propagator

$$G^{\mathrm{F}/\overline{\mathrm{F}}}(x^0, \vec{x}) = \pm \mathrm{i} G^{\mathrm{E}}(\pm \mathrm{i} x^0, \vec{x}). \tag{4.24}$$

We obtain (4.21). This is obvious for spacelike $x^0, \vec{x}$, where the Wick rotation does not change the sign of x^2 and therefore we still obtain an expression involving the Macdonald function. Inside the light cones the sign of x^2 changes. More precisely, we can interpret the Wick rotation as $\mathrm{e}^{\pm \mathrm{i}\phi} x^0$ with $\phi \in [0, \frac{\pi}{2}]$ and we obtain expressions involving Hankel functions. For $\phi \in]0, \frac{\pi}{2}[$ we have $\pm \mathrm{Im}\big((\mathrm{e}^{\pm \mathrm{i}\phi} x^0)^2 + (\vec{x})^2\big) > 0$. Therefore, the Eclidean square $|x|^2$ has to be replaced with the Lorentzian square $x^2 \pm \mathrm{i}0$. On the surface of the light cone the terms involving u, v are sufficiently regular and cause no problem. However the function $\frac{1}{|x|^2}$ becomes

$$\frac{1}{x^2 \pm \mathrm{i}0} = \frac{1}{x^2} \mp \mathrm{i}\pi \delta(x^2) = \frac{1}{x^2} \mp \frac{\mathrm{i}\pi}{2|\vec{x}|} \big(\delta(x^0 + |\vec{x}|) + \delta(x^0 - |\vec{x}|) \big), \tag{4.25}$$

where we used the Sochocki formula and $\frac{1}{x^2}$ is meant in terms of the principal value.

Then we compute

$$G^{\vee}(x) + G^{\wedge}(x) = G^{\mathrm{F}}(x) + G^{\overline{\mathrm{F}}}(x) \tag{4.26}$$

$$= \frac{1}{2\pi} \delta(x^2) - \frac{m\theta(-x^2)}{4\pi\sqrt{-x^2}} J_1(m\sqrt{-x^2}). \tag{4.27}$$

Now we can obtain the forward/backward propagators from

$$G^{\vee/\wedge} = \theta(\pm x^0) \big(G^{\mathrm{F}}(x) + G^{\overline{\mathrm{F}}}(x) \big). \tag{4.28}$$

Finally, we can read off the formulas for positive/negative frequency solutions from (4.17).

Below we give the formulas for the massless propagators in the position representation in dimension $1 + 3$.

- The forward/backward propagator:

$$G^{\vee/\wedge}(x) \quad = \quad \frac{1}{2\pi}\theta(\pm x^0)\delta(x^2) = \frac{\delta(x^0 \mp |\vec{x}|)}{4\pi|\vec{x}|}.$$

- The *(anti-)Feynman propagator*:

$$G^{\mathrm{F}/\overline{\mathrm{F}}}(x) \quad = \quad \frac{\pm \mathrm{i}}{4\pi^2(x^2 \pm \mathrm{i}0)}.$$

- The *Pauli-Jordan* or the *commutator function*:

$$G^{\mathrm{PJ}}(x) \quad = \quad \frac{1}{2\pi}\mathrm{sgn}x^0\delta(x^2) = \frac{\delta(x^0 - |\vec{x}|)}{4\pi|\vec{x}|} - \frac{\delta(x^0 + |\vec{x}|)}{4\pi|\vec{x}|}.$$

- The *positive frequency*, resp. *negative frequency*:

$$G^{(\pm)}(x) \quad = \quad \frac{1}{4\pi(x^2 \pm \mathrm{i}0\mathrm{sgn}x^0)}.$$

4.6 Classical propagators and solving the Klein-Gordon equation

A function on $\mathbb{R}^{1,n}$ is called *space compact* if there exists a compact $K \subset \mathbb{R}^{1,n}$ such that $\mathrm{supp}f \subset J(K)$. It is called *future/past space-compact* if there exists a compact $K \subset \mathbb{R}^{1,n}$ such that $\mathrm{supp}f \subset J^{\pm}(K)$.

The set of space compact smooth functions will be denoted $C^{\infty}_{\mathrm{sc}}(\mathbb{R}^{1,n})$.

Proposition 4.3. *Let $f \in C^{\infty}_{\mathrm{c}}(\mathbb{R}^{1,n})$.*

(1) *$\zeta^{\vee/\wedge}(x) := \int G^{\vee/\wedge}(x-y)f(y)\mathrm{d}y$ is the unique solution of*

$$(-\Box + m^2)\zeta = f. \tag{4.29}$$

future/past space compact.

(2) *$\zeta(x) := \int G^{\mathrm{PJ}}(x-y)f(y)\mathrm{d}y$ is a solution of*

$$(-\Box + m^2)\zeta = 0. \tag{4.30}$$

Every smooth space-compact solution of (4.30) is of this form.

$G^{\mathrm{PJ}}(x)$ is the unique solution of the Klein-Gordon equation satisfying

$$G^{\mathrm{PJ}}(0,\vec{x}) = 0, \ \dot{G}^{\mathrm{PJ}}(0,\vec{x}) = \delta(\vec{x}). \tag{4.31}$$

Proposition 4.4. *Let $\alpha, \beta \in C^{\infty}_{\mathrm{c}}(\mathbb{R}^n)$. Then there exists a unique $\zeta \in C^{\infty}_{\mathrm{sc}}(\mathbb{R}^{1,n})$ that solves*

$$(-\Box + m^2)\zeta = 0 \tag{4.32}$$

with initial conditions $\zeta(0,\vec{x}) = \alpha(\vec{x}), \quad \dot{\zeta}(0,\vec{x}) = \beta(\vec{x})$. It satisfies $\mathrm{supp}\zeta \subset J(\mathrm{supp}\alpha \cup \mathrm{supp}\beta)$ and is given by

$$\zeta(t,\vec{x}) \quad = \quad \int_{\mathbb{R}^n} \dot{G}^{\mathrm{PJ}}(t,\vec{x}-\vec{y})\alpha(\vec{y})\mathrm{d}\vec{y} + \int_{\mathbb{R}^n} G^{\mathrm{PJ}}(t,\vec{x}-\vec{y})\beta(\vec{y})\mathrm{d}\vec{y}. \tag{4.33}$$

Proof. Clearly, (4.33) satisfies (4.32). Using (4.31) we check that $\zeta(0,\vec{x}) = \alpha(\vec{x})$. We have

$$\ddot{G}^{\mathrm{PJ}}(0,\vec{x}) = (\Delta - m^2)G^{\mathrm{PJ}}(0,\vec{x}) = 0. \tag{4.34}$$

Now we can verify that $\dot{\zeta}(0,\vec{x}) = \beta(\vec{x})$. □

5 Second quantization

In this chapter we describe the terminology and notation of multilinear algebra. We will concentrate on the infinite dimensional case, where it is often natural to use the structure of Hilbert spaces. We will introduce Fock spaces and various classes of operators acting on them. In quantum physics the passage from a dynamics on one-particle spaces to a dynamics on Fock spaces is often called *second quantization* – hence the name of the chapter.

We will consider two setups: that of vector spaces and that of Hilbert spaces. If $\mathcal{X}, \mathcal{Y}$ are vector spaces, then $L(\mathcal{X}, \mathcal{Y})$ will denote the set of linear operators from $\mathcal{X}$ to $\mathcal{Y}$. If $\mathcal{X}, \mathcal{Y}$ are Hilbert spaces, then $B(\mathcal{X}, \mathcal{Y})$ will denote the set of bounded operators fro $\mathcal{X}$ to $\mathcal{Y}$.

5.1 Vector and Hilbert spaces

Let $\mathcal{V}$ be a vector space. A set $\{e_i \ : \ i \in I\} \subset \mathcal{V}$ is called linearly independent if for any finite subset $\{e_{i_1}, \dots, e_{i_n}\} \subset \{e_i \ : \ i \in I\}$

$$c_1 e_{i_1} + \cdots + c_n e_{i_n} = 0 \quad \Rightarrow \quad c_1 = \cdots = c_n = 0. \tag{5.1}$$

$\{e_i \ : \ i \in I\}$ is a Hamel basis (or simply a basis) of $\mathcal{V}$ if it is a maximal linearly independent set. It means that it is linearly independent and if we add any $v \in \mathcal{V}$ to $\{e_i \ : \ i \in I\} \subset \mathcal{V}$ then it is not linearly independent any more. Note that every $v \in \mathcal{V}$ can be written as a finite linear combination $v = \sum_{i \in I} \lambda_i e_i$ in a unique way.

Let $\mathcal{V}$ be a vector space over $\mathbb{C}$ or $\mathbb{R}$ equipped with a scalar product $(v|w)$ (positive, nondegenerate, sesquilinear form). It defines a metric on $\mathcal{V}$ by

$$\|v - w\| := \sqrt{(v - w|v - w)}. \tag{5.2}$$

We say that $\mathcal{V}, (\cdot|\cdot)$ is a Hilbert space if $\mathcal{V}$ is complete.

If $\mathcal{V}, (\cdot|\cdot)$ is not necessarily complete, then we can always complete it, that is find a larger complete space $\mathcal{V}^{\mathrm{cpl}}, (\cdot|\cdot)$ in which $\mathcal{V}$ is embedded as a dense subspace. $\mathcal{V}^{\mathrm{cpl}}$ is uniquely defined and is called the completion of $\mathcal{V}$.

For instance, if we take $C_{\mathrm{c}}(\mathbb{R})$, $C_{\mathrm{c}}^{\infty}(\mathbb{R})$ or $\mathcal{S}(\mathbb{R})$ with the usual scalar product $(f|g) = \int \overline{f(x)} g(x) \mathrm{d}x$, then its completion is $L^2(\mathbb{R})$.

If $\mathcal{V}$ is a Hilbert space, then $\{e_i \ : \ i \in I\}$ is called an orthonormal basis (o.n.b.) if it is a maximal orthonormal set. Note that every $v \in \mathcal{V}$ can be written as a linear combination $v = \sum_{i \in I} \lambda_i e_i$, where $\sum_{i \in I} |\lambda_i|^2 < \infty$, in a unique way

Note that in a finite dimensional Hilbert space every orthonormal basis is a basis. This is not true in infinite dimensional Hilbert spaces.

5.2 Direct sum

Let $(\mathcal{V}_i)_{i\in I}$ be a family of vector spaces. The *algebraic direct sum of* $\mathcal{V}_i$ will be denoted

$$\overset{\text{al}}{\bigoplus_{i\in I}} \mathcal{V}_i, \tag{5.3}$$

It consists of sequences $(v_i)_{i\in I}$, which are zero for all but a finite number of elements.

If $(\mathcal{V}_i)_{i\in I}$ is a family of Hilbert spaces, then $\overset{\text{al}}{\bigoplus_{i\in I}} \mathcal{V}_i$ has a natural scalar product.

$$\Big((y_i)_{i\in I}\Big|(v_i)_{i\in I}\Big) = \sum_{i\in I}(y_i|v_i). \tag{5.4}$$

The *direct sum of* $\mathcal{V}_i$ *in the sense of Hilbert spaces* is defined as

$$\bigoplus_{i\in I} \mathcal{V}_i := \left(\overset{\text{al}}{\bigoplus_{i\in I}} \mathcal{V}_i\right)^{\text{cpl}}.$$

If I is finite, then $\overset{\text{al}}{\bigoplus_{i\in I}} \mathcal{V}_i = \bigoplus_{i\in I} \mathcal{V}_i$

Let $(\mathcal{V}_i)$, $(\mathcal{W}_i)$, $i \in I$, be families of vector spaces. If $a_i \in L(\mathcal{V}_i, \mathcal{W}_i)$, $i \in I$, then their *direct sum* is denoted $\bigoplus_{i\in I} a_i$ and belongs to $L\left(\overset{\text{al}}{\bigoplus_{i\in I}} \mathcal{V}_i, \overset{\text{al}}{\bigoplus_{i\in I}} \mathcal{W}_i\right)$. It is defined as

$$\Big(\bigoplus_{i\in I} a_i\Big)(v_i)_{i\in I} = (a_i v_i)_{i\in I} \tag{5.5}$$

Let $\mathcal{V}_i$, $\mathcal{W}_i$, $i \in I$ be families of Hilbert spaces, and $a_i \in B(\mathcal{V}_i, \mathcal{W}_i)$ with $\sup_{i\in I} \|a_i\| < \infty$. Then the operator $\bigoplus_{i\in I} a_i$ is bounded. Its extension in $B\left(\bigoplus_{i\in I} \mathcal{V}_i, \bigoplus_{i\in I} \mathcal{W}_i\right)$ will be denoted by the same symbol.

5.3 Tensor product

Let $\mathcal{V}, \mathcal{W}$ be vector spaces. The *algebraic tensor product of* $\mathcal{V}$ *and* $\mathcal{W}$ will be denoted $\mathcal{V} \overset{\text{al}}{\otimes} \mathcal{W}$. Here is one of its definitions

Let $\mathcal{Z}$ be the space of finite linear combinations of vectors (v, w), $v \in \mathcal{V}$, $w \in \mathcal{W}$. In $\mathcal{Z}$ we define the subspace $\mathcal{Z}_0$ spanned by

$$\begin{aligned} (\lambda v, w) - \lambda(v, w), \qquad & (v, \lambda w) - \lambda(v, w), \\ (v_1 + v_2, w) - (v_1, w) - (v_2, w), \qquad & (v, w_1 + w_2) - (v, w_1) - (v, w_2). \end{aligned}$$

We set $\mathcal{V} \overset{\text{al}}{\otimes} \mathcal{W} := \mathcal{Z}/\mathcal{Z}_0$. If $v \in \mathcal{V}$, $w \in \mathcal{W}$, we define $v \otimes w := (v, w) + \mathcal{Z}_0$.

Remark 5.1. *Note that* (v, w) *above is just a symbol and not an element of* $\mathcal{V} \oplus \mathcal{W}$. *Elements of the space* $\mathcal{Z}$ *have the form*

$$\sum_{j=1}^{n} \lambda_n(v_n, w_n). \tag{5.6}$$

In particular, in general

$$(v_1, w_1) + (v_2, w_2) \not\sim (v_1 + v_2, w_1 + w_2), \tag{5.7}$$
$$\lambda(v, w) \not\sim (\lambda v, \lambda w). \tag{5.8}$$

$\mathcal{V} \overset{\text{al}}{\otimes} \mathcal{W}$ is a vector space and $\otimes$ is an operation satisfying

$$(\lambda v) \otimes w = \lambda v \otimes w, \qquad v \otimes (\lambda w) = \lambda v \otimes w,$$
$$(v_1 + v_2) \otimes w = v_1 \otimes w + v_2 \otimes w, \qquad v \otimes (w_1 + w_2) = v \otimes w_1 + v \otimes w_2.$$

Vectors of the form $v \otimes w$ are called *simple tensors*. Not all elements of $\mathcal{V} \otimes \mathcal{W}$ are simple tensors, but they span $\mathcal{V} \overset{\text{al}}{\otimes} \mathcal{W}$.

If $\{e_i\}_{i\in I}$ and $\{f_j\}_{j\in J}$ are bases of $\mathcal{V}$, resp. $\mathcal{W}$, then $\{e_i \otimes f_j\}_{(i,j)\in I\times J}$ is a basis of $\mathcal{V} \overset{\text{al}}{\otimes} \mathcal{W}$,

If $\mathcal{V}$, $\mathcal{W}$ are Hilbert spaces, then $\mathcal{V} \overset{\text{al}}{\otimes} \mathcal{W}$ has a unique scalar product such that

$$(v_1 \otimes w_1 | v_2 \otimes w_2) := (v_1|v_2)(w_1|w_2), \quad v_1, v_2 \in \mathcal{V}, \quad w_1, w_2 \in \mathcal{W}.$$

To see this it is enough to choose o.n.b's $\{e_i\}_{i\in I}$ and $\{f_j\}_{j\in J}$ in $\mathcal{V}$, resp. $\mathcal{W}$. Then every element of $\mathcal{V} \overset{\text{al}}{\otimes} \mathcal{W}$ can be written as an (infinite) linear combination of $e_i \otimes f_j$ and we can use them as an orthonormal set defining this scalar product.

We set

$$\mathcal{V} \otimes \mathcal{W} := (\mathcal{V} \overset{\text{al}}{\otimes} \mathcal{W})^{\text{cpl}},$$

and call it the *tensor product of $\mathcal{V}$ and $\mathcal{W}$ in the sense of Hilbert spaces*. If $\{e_i\}_{i\in I}$ and $\{f_j\}_{j\in J}$ are o.n.b's of $\mathcal{V}$, resp. $\mathcal{W}$, then $\{e_i \otimes f_j\}_{(i,j)\in I\times J}$ is an o.n.b. of $\mathcal{V} \otimes \mathcal{W}$,

If one of the spaces $\mathcal{V}$ or $\mathcal{W}$ is finite dimensional, then $\mathcal{V} \overset{\text{al}}{\otimes} \mathcal{W} = \mathcal{V} \otimes \mathcal{W}$.

Let $\mathcal{V}_1, \mathcal{V}_2, \mathcal{W}_1, \mathcal{W}_2$ be vector spaces. If $a \in L(\mathcal{V}_1, \mathcal{V}_2)$ and $b \in L(\mathcal{W}_1, \mathcal{W}_2)$, then there exists a unique operator $a \otimes b \in L(\mathcal{V}_1 \overset{\text{al}}{\otimes} \mathcal{W}_1, \mathcal{V}_2 \overset{\text{al}}{\otimes} \mathcal{W}_2)$ such that on simple tensors we have

$$(a \otimes b)(y \otimes w) = (ay) \otimes (bw). \tag{5.9}$$

To see this it is enough to choose bases $(e_i)_{i\in I}$ in $\mathcal{V}_1$ and $(f_j)_{j\in J}$ in $\mathcal{W}_1$ and to define $a \otimes b$ on the basis $(e_i \otimes f_j)_{(i,j)\in I\times J}$ by

$$(a \otimes b)e_i \otimes f_j := (ae_i) \otimes (bf_j). \tag{5.10}$$

Then we check that thus defined operator satisfies (5.9) and is unique. It is called the *tensor product of a and b*.

If $\mathcal{V}_1, \mathcal{V}_2, \mathcal{W}_1, \mathcal{W}_2$ are Hilbert spaces and $a \in B(\mathcal{V}_1, \mathcal{V}_2)$, $b \in B(\mathcal{W}_1, \mathcal{W}_2)$, then $a \otimes b$ is bounded. It extends uniquely to an operator in $B(\mathcal{V}_1 \otimes \mathcal{W}_1, \mathcal{V}_2 \otimes \mathcal{W}_2)$, denoted by the same symbol.

To prove the boundedness of $a \otimes b = a \otimes \mathbb{1}\ \mathbb{1} \otimes b$, it is sufficient to consider the operator $a \otimes \mathbb{1}$ from $\mathcal{V}_1 \overset{\text{al}}{\otimes} \mathcal{W}$ to $\mathcal{V}_2 \overset{\text{al}}{\otimes} \mathcal{W}$. Let $e_1, e_2, \dots$ and $f_1, f_2 \dots$ be orthonormal bases in $\mathcal{V}_1$, $\mathcal{W}$ resp. Consider a vector $\sum c_{ij} \mathrm{e}_i \otimes f_j$.

$$\begin{aligned} \Big\| a \otimes \mathbb{1} \sum_i c_{ij} e_i \otimes f_j \Big\|^2 &= \sum_j \Big\| \sum_i c_{ij} a e_i \Big\|^2 \\ \leq \sum_j \|a\|^2 \Big\| \sum_i c_{ij} e_i \Big\|^2 &\leq \sum_j \|a\|^2 \sum_i |c_{ij}|^2 \\ &= \|a\|^2 \Big\| \sum_{ij} c_{ij} e_i \otimes f_j \Big\|^2. \end{aligned}$$

5.4 Fock spaces

Let $\mathcal{Y}$ be a vector space. Let S_n denote the *permutation group of n elements* and $\sigma \in S_n$. $\Theta(\sigma)$ is defined as the unique operator in $L(\overset{\text{al}}{\otimes}{}^n \mathcal{Y})$ such that

$$\Theta(\sigma) y_1 \otimes \cdots \otimes y_n = y_{\sigma^{-1}(1)} \otimes \cdots \otimes y_{\sigma^{-1}(n)}. \tag{5.11}$$

To see that $\Theta(\sigma)$ is well defined we first choose a basis $\{e_i\}_{i \in I}$ of $\mathcal{Y}$. Then we define $\Theta(\sigma)$ on the corresponding basis of $\overset{\text{al}}{\otimes}{}^n \mathcal{Y}$:

$$\Theta(\sigma) e_{i_1} \otimes \cdots \otimes e_{i_n} = e_{i_{\sigma^{-1}(1)}} \otimes \cdots \otimes e_{i_{\sigma^{-1}(n)}}.$$

Then we extend by linearity $\Theta(\sigma)$ to the whole $\overset{\text{al}}{\otimes}{}^n \mathcal{Y}$. It is easy to see that the operator defined in this way satisfies (5.11).

We can check that

$$S_n \ni \sigma \mapsto \Theta(\sigma) \in L(\overset{\text{al}}{\otimes}{}^n \mathcal{Y}) \tag{5.12}$$

is a group representation.

We say that a tensor $\Psi \in \overset{\text{al}}{\otimes}{}^n \mathcal{Y}$ is symmetric, resp. antisymmetric if

$$\Theta(\sigma)\Psi = \Psi, \tag{5.13}$$

$$\text{resp.} \qquad \Theta(\sigma)\Psi = \operatorname{sgn}(\sigma)\Psi. \tag{5.14}$$

We define the *symmetrization/antisymmetrization projections*

$$\Theta^n_{\text{s}} := \frac{1}{n!} \sum_{\sigma \in S_n} \Theta(\sigma), \qquad \Theta^n_{\text{a}} := \frac{1}{n!} \sum_{\sigma \in S_n} \operatorname{sgn}\sigma \Theta(\sigma).$$

They project onto symmetric/antisymmetric tensors.

We will often write s/a to denote either s or a.

If $\mathcal{Y}$ is a Hilbert space, then $\Theta(\sigma)$ is unitary and $\Theta^n_{\text{s/a}}$ are orthogonal projections.

Let $\mathcal{Y}$ be a vector space. The *algebraic n-particle bosonic/fermionic space* is defined as

$$\overset{\text{al}}{\otimes}{}^n_{\text{s/a}} \mathcal{Y} := \Theta^n_{\text{s/a}} \overset{\text{al}}{\otimes}{}^n \mathcal{Y}.$$

The *algebraic bosonic/fermionic Fock space* or the *symmetric/antisymmetric tensor algebra* is

$$\overset{\text{al}}{\Gamma}_{\text{s/a}}(\mathcal{Y}) := \overset{\infty}{\underset{n=0}{\overset{\text{al}}{\oplus}}} \overset{\text{al}}{\otimes}{}^n_{\text{s/a}}\mathcal{Y}.$$

The *vacuum vector* is $\Omega := 1 \in \otimes^0_{\text{s/a}}\mathcal{Y} = \mathbb{C}$.

If $\mathcal{Y}$ is a Hilbert space, then the *n-particle bosonic/fermionic space* is defined as

$$\otimes^n_{\text{s/a}}\mathcal{Y} := \Theta^n_{\text{s/a}} \otimes^n \mathcal{Y}.$$

The *bosonic/fermionic Fock space* is

$$\Gamma_{\text{s/a}}(\mathcal{Y}) := \overset{\infty}{\underset{n=0}{\oplus}} \otimes^n_{\text{s/a}}\mathcal{Y}.$$

5.5 Creation/annihilation operators

For $z \in \mathcal{Y}$ we define the *creation operator*

$$\hat{a}^*(z)\Psi := \Theta^{n+1}_{\text{s/a}}\sqrt{n+1}z \otimes \Psi, \quad \Psi \in \otimes^n_{\text{s/a}}\mathcal{Y},$$

and the *annihilation operator* $\hat{a}(z) := (\hat{a}^*(z))^*$. (We often omit the hat).

We will sometimes write $(z|$ and $|z)$ for the following operators

$$\mathcal{V} \ni v \mapsto (z|v := (z|v) \in \mathbb{C}, \tag{5.15}$$

$$\mathbb{C} \ni \lambda \mapsto \lambda|z) := \lambda z \in \mathcal{V}. \tag{5.16}$$

Then on $\otimes^n_{\text{s/a}}\mathcal{Y}$ we have

$$a^*(z) = \Theta^{n+1}_{\text{s/a}}\sqrt{n+1}|z) \otimes \mathbb{1}^{n\otimes}, \tag{5.17}$$

$$a(z) = \sqrt{n}(z| \otimes \mathbb{1}^{(n-1)\otimes}. \tag{5.18}$$

Above we used the *compact notation* for creation/annihilation operators popular among mathematicians. Physicists commonly prefer the *traditional notation*, which is longer and less canonical.

One version of the traditional notation uses a fixed basis $\{e_i\}_{i\in I}$ of $\mathcal{Z}$ and set $a^*_i := a^*(e_i)$, $a_i := a(e_i)$. Then if $z = \sum_i z_i e_i$, we have

$$a^*(z) = \sum_i z_i a^*_i, \quad a(z) = \sum_i \overline{z}_i a_i, \tag{5.19}$$

$$[a_i, a^*_j]_\mp = \delta_{ij}, \quad [a_i, a_j]_\mp = 0. \tag{5.20}$$

Alternatively, one often identifies $\mathcal{Z}$ with, say, $L^2(\mathbb{R}^d, \mathrm{d}\xi)$. If z equals a function $\Xi \ni \xi \mapsto z(\xi)$, then

$$a^*(z) = \int z(\xi)a^*_\xi \mathrm{d}\xi, \quad a(z) = \int \overline{z}(\xi)a_\xi \mathrm{d}\xi.$$

Note that formally

$$[a(\xi), a^*(\xi')]_\mp = \delta(\xi - \xi'), \quad [a(\xi), a(\xi')]_\mp = 0. \tag{5.21}$$

The space $\otimes^n_{\mathrm{s/a}} \mathcal{Z}$ can then be identified with the space of symmetric/antisymmetric square integrable functions $L^2(\mathbb{R}^{nd})$, and then

$$\big(a(\xi)\Phi\big)(\xi'_1, \dots, \xi'_{n-1}) = \sqrt{n}\Phi(\xi, \xi'_1, \dots, \xi'_{n-1}). \tag{5.22}$$

5.6 Integral kernel of an operator

Every linear operator A on $\mathbb{C}^n$ can be represented by a matrix $[A^j_i]$.

One would like to generalize this concept to infinite dimensional spaces (say, Hilbert spaces) and continuous variables instead of a discrete variables i, j. Suppose that a given vector space is represented, say, as $L^2(\mathbb{R}^d)$, or more generally, $L^2(X)$ where X is a certain space with a measure. One often uses the representation of an operator A in terms of its *integral kernel* $\mathbb{R}^d \times \mathbb{R}^d \ni (x, y) \mapsto A(x, y)$, so that

$$A\Psi(x) = \int A(x, y)\Psi(y)\mathrm{d}y.$$

Note that strictly speaking $A(\cdot, \cdot)$ does not have to be a function. E.g. in the case $X = \mathbb{R}^d$ it could be a distribution, hence one often says the *distributional kernel* instead of the *integral kernel*. Sometimes $A(\cdot, \cdot)$ is ill-defined anyway. At least formally, we have

$$AB(x, y) = \int A(x, z)B(z, y)\mathrm{d}z,$$

$$A^*(x, y) = \overline{A(y, x)}.$$

Here is a situation where there is a good mathematical theory of integral/distributional kernels:

Theorem 5.2 (The Schwartz kernel theorem)**.** *B is a continuous linear transformation from $\mathcal{S}(\mathbb{R}^d)$ to $\mathcal{S}'(\mathbb{R}^d)$ iff there exists a distribution $B(\cdot, \cdot) \in \mathcal{S}'(\mathbb{R}^d \oplus \mathbb{R}^d)$ such that*

$$(\Psi | B\Phi) = \int \overline{\Psi(x)}B(x, y)\Phi(y)\mathrm{d}x\mathrm{d}y, \quad \Psi, \Phi \in \mathcal{S}(\mathbb{R}^d).$$

Note that $\Leftarrow$ is obvious. The distribution $B(\cdot, \cdot) \in \mathcal{S}'(\mathbb{R}^d \oplus \mathbb{R}^d)$ is called the *distributional kernel of the transformation B*. All bounded operators on $L^2(\mathbb{R}^d)$ satisfy the Schwartz kernel theorem.

Examples:

(1) $\mathrm{e}^{-\mathrm{i}xy}$ is the kernel of the Fourier transformation

(2) $\delta(x - y)$ is the kernel of identity.

(3) $\partial_x \delta(x - y)$ is the kernel of ∂_x.

5.7 Second quantization of operators

For a contraction q on $\mathcal{Z}$ the operator $q^{\otimes n}$ commutes with $\Theta(\sigma)$, $\sigma \in S_n$. Therefore, it preserves $\otimes^n_{\mathrm{s/a}}\mathcal{Z}$. We define the operator $\Gamma(q)$ on $\Gamma_{\mathrm{s/a}}(\mathcal{Z})$ by

$$\Gamma(q)\Big|_{\otimes^n_{\mathrm{s/a}}\mathcal{Z}} = q \otimes \cdots \otimes q\Big|_{\otimes^n_{\mathrm{s/a}}\mathcal{Z}}.$$

$\Gamma(q)$ is called the *second quantization of* q.

Similarly, for an operator h on $\mathcal{Z}$ the operator $h\otimes 1^{(n-1)\otimes} + \cdots + 1^{(n-1)\otimes}\otimes h$ preserves $\otimes^n_{\mathrm{s/a}}\mathcal{Z}$. We define the operator $\mathrm{d}\Gamma(h)$ by

$$\mathrm{d}\Gamma(h)\Big|_{\otimes^n_{\mathrm{s/a}}\mathcal{Z}} = h \otimes 1^{(n-1)\otimes} + \cdots + 1^{(n-1)\otimes} \otimes h\Big|_{\otimes^n_{\mathrm{s/a}}\mathcal{Z}}.$$

$\mathrm{d}\Gamma(h)$ is called the *(infinitesimal) second quantization of* h.

Note the identities

$$\begin{aligned}&\Gamma(\mathrm{e}^{\mathrm{i}th}) = \mathrm{e}^{\mathrm{i}t\mathrm{d}\Gamma(h)}, \quad \Gamma(q)\Gamma(r) = \Gamma(qr), \quad [\mathrm{d}\Gamma(h), \mathrm{d}\Gamma(k)] = \mathrm{d}\Gamma([h,k]),\\ &\Gamma(q)\mathrm{d}\Gamma(h)\Gamma(q^{-1} = \mathrm{d}\Gamma(qhq^{-1}).\end{aligned} \tag{5.23}$$

Let $\{e_i \mid i \in I\}$ be an orthonormal basis of $\mathcal{Z}$. Write $\hat{a}_i := \hat{a}(e_i)$. Let h be an operator on $\mathcal{Z}$ given by the matrix $[h_{ij}]$. Then

$$\mathrm{d}\Gamma(h) = \sum_{ij} h_{ij}\hat{a}_i^*\hat{a}_j. \tag{5.24}$$

Let us prove it in the bosonic case. Let $\Phi \in \Gamma^n_{\mathrm{s}}(\mathcal{Z})$.

$$\hat{a}_i^*\hat{a}_j\Phi = n\Theta^n_{\mathrm{s}}|e_i) \otimes \mathbb{1}^{(n-1)\otimes}(e_j| \otimes \mathbb{1}^{(n-1)\otimes}\Phi \tag{5.25}$$

$$= n\Theta^n_{\mathrm{s}}|e_i)(e_j| \otimes \mathbb{1}^{(n-1)\otimes}\Phi \tag{5.26}$$

$$= \frac{1}{(n-1)!}\sum_{\sigma\in S_n} \Theta(\sigma)|e_i)(e_j| \otimes \mathbb{1}^{(n-1)\otimes}\Theta(\sigma)^{-1}\Phi \tag{5.27}$$

$$= \sum_{k=1}^{n} \mathbb{1}^{(k-1)\otimes}|e_i)(e_j| \otimes \mathbb{1}^{(n-k)\otimes}\Phi. \tag{5.28}$$

More generally, if the integral kernel of an operator h is $h(x,y)$, then

$$\mathrm{d}\Gamma(h) = \int h(x,y)\hat{a}_x^*\hat{a}_y\mathrm{d}x\mathrm{d}y. \tag{5.29}$$

For instance, if h is the multiplication operator by $h(\xi)$, then $\mathrm{d}\Gamma(h) = \int h(\xi)\hat{a}_\xi^*\hat{a}_\xi\mathrm{d}\xi$.

5.8 Symmetric/antisymmetric tensor product

Let $\Psi \in \otimes^p_{\mathrm{s/a}}\mathcal{Z}$, $\Phi \in \otimes^q_{\mathrm{s/a}}\mathcal{Z}$. We set

$$\Psi \otimes_{\mathrm{s/a}} \Phi := \Theta^{p+q}_{\mathrm{s/a}}\Psi \otimes \Phi. \tag{5.30}$$

Note that

$$z \otimes \cdots \otimes z = z \otimes_{\mathrm{s}} \cdots \otimes_{\mathrm{s}} z. \tag{5.31}$$

If there are n terms, it is often written as $z^{n\otimes}$. In the antisymmetric case one usually prefers

$$\Psi \wedge \Phi := \frac{(p+q)!}{p!q!} \Psi \otimes_{\mathrm{a}} \Phi. \tag{5.32}$$

The operations $\otimes_{\mathrm{s}}$, $\otimes_{\mathrm{a}}$, $\wedge$ are associative. We have

$$y_1 \wedge \cdots \wedge y_n = \sum_{\sigma \in S_n} \operatorname{sgn}(\sigma) y_{\sigma(1)} \otimes \cdots \otimes y_{\sigma(n)}, \tag{5.33}$$

$$y_1 \otimes_{\mathrm{a}} \cdots \otimes_{\mathrm{a}} y_n = \frac{1}{n!} \sum_{\sigma \in S_n} \operatorname{sgn}(\sigma) y_{\sigma(1)} \otimes \cdots \otimes y_{\sigma(n)}. \tag{5.34}$$

Let $\{e_i\}_{i \in I}$ be a linearly ordered orthonormal basis in $\mathcal{Z}$. Then

$$\sqrt{n!} e_{i_1} \otimes_{\mathrm{a}} \cdots \otimes_{\mathrm{a}} e_{i_n}, \quad i_1 < \cdots < i_n, \tag{5.35}$$

forms an o.n.b of $\otimes^n_{\mathrm{a}}(\mathcal{Z})$.

$$\frac{\sqrt{n!}}{\sqrt{k_1! \cdots k_n!}} e_{i_1}^{\otimes k_1} \otimes_{\mathrm{s}} \cdots \otimes_{\mathrm{s}} e_{i_m}^{\otimes k_m}, \quad k_1 + \cdots + k_m = n, \tag{5.36}$$

forms an o.n.b of $\otimes^m_{\mathrm{s}}(\mathcal{Z})$.

If $\dim \mathcal{Z} = d$, then

$$\dim \otimes^n_{\mathrm{s}} \mathcal{Z} = \frac{(d+n-1)!}{(d-1)!n!}, \quad \dim \otimes^n_{\mathrm{a}} \mathcal{Z} = \frac{d!}{n!(d-n)!}. \tag{5.37}$$

5.9 Exponential law

Let $\mathcal{Z}, \mathcal{W}$ be Hilbert spaces. We can treat them as subspaces of $\mathcal{Z} \oplus \mathcal{W}$. Let $\Phi \in \otimes^n_{\mathrm{s/a}} \mathcal{Z}$, $\Psi \in \otimes^m_{\mathrm{s/a}} \mathcal{W}$. We can identify $\Phi \otimes \Psi$ with

$$U\Phi \otimes \Psi := \sqrt{\frac{(n+m)!}{n!m!}} \Phi \otimes_{\mathrm{s/a}} \Psi \in \otimes^{n+m}_{\mathrm{s/a}}(\mathcal{Z} \oplus \mathcal{W}). \tag{5.38}$$

Theorem 5.3. *The map* (5.38) *extends to a unitary map*

$$U : \Gamma_{\mathrm{s/a}}(\mathcal{Z}) \otimes \Gamma_{\mathrm{s/a}}(\mathcal{W}) \to \Gamma_{\mathrm{s/a}}(\mathcal{Z} \oplus \mathcal{W}). \tag{5.39}$$

It satisfies

$$U\Omega \otimes \Omega = \Omega, \tag{5.40}$$

$$\mathrm{d}\Gamma(h \oplus g)U = U\big(\mathrm{d}\Gamma(h) \otimes \mathbb{1} + \mathbb{1} \otimes \mathrm{d}\Gamma(g)\big), \tag{5.41}$$

$$\Gamma(p \oplus q)U = U\Gamma(p) \otimes U\Gamma(q), \tag{5.42}$$

$$a^*(z \oplus w)U = U\big(a^*(z) \otimes \mathbb{1} + \mathbb{1} \otimes a^*(w)\big), \tag{5.43}$$

$$a(z \oplus w)U = U\big(a(z) \otimes \mathbb{1} + \mathbb{1} \otimes a(w)\big), \quad \textit{in the bosonic case}, \tag{5.44}$$

$$a^*(z \oplus w)U = U\big(a^*(z) \otimes \mathbb{1} + (-1)^N \otimes a^*(z)\big), \tag{5.45}$$

$$a(z \oplus w)U = U\big(a(z) \otimes \mathbb{1} + (-1)^N \otimes a(z)\big), \quad \textit{in the fermionic case}. \tag{5.46}$$

Proof. Let us prove the unitarity of this map in the symmetric case:

$$\Phi \otimes_{\rm s} \Psi = \frac{1}{(n+m)!} \sum_{\sigma \in S_{n+m}} \Theta(\sigma)\Phi \otimes \Psi \tag{5.47}$$

$$= \frac{n!m!}{(n+m)!} \sum_{[\sigma] \in S_{n+m}/S_n \times S_m} \Theta(\sigma)\Phi \otimes \Psi. \tag{5.48}$$

The terms on the right are mutually orthogonal. The maps $\Theta(\sigma)$ are unitary. The number of cosets in $S_{n+m}/S_n \times S_m$ is $\frac{(n+m)!}{n!m!}$. Therefore the square norm of (5.47) is

$$\frac{n!m!}{(n+m)!} \|\Phi \otimes \Psi\|^2. \tag{5.49}$$

□

5.10 Wick symbol

Let $\mathcal{Z} = L^2(\mathbb{R}^d)$ or $\mathcal{Z} = \mathbb{C}^n$. The variable ξ will be interpreted as an elemenrt of $\mathbb{R}^d$ in the former case, as $\xi = 1, 2, \dots, n$ in the latter case. $\int \mathrm{d}\xi$ will have the usual meaning in the first case, it will be $\sum_{\xi=1}^n$ in the second.

$$(\xi_1, \cdots \xi_m, \xi'_k, \cdots, \xi'_1) \mapsto b(\xi_1, \cdots \xi_m, \xi'_k, \cdots, \xi'_1) \tag{5.50}$$

be a complex function. Note that (5.50) can be also interpreted as the integral kernel of an operator b from $\otimes^k \mathcal{Z}$ to $\otimes^m \mathcal{Z}$:

$$(\Phi|b\Psi) = \int \cdots \int \overline{\Phi(\xi_1, \cdots \xi_m)} b(\xi_1, \cdots \xi_m, \xi'_k, \cdots, \xi'_1)$$
$$\Psi(\xi'_k, \cdots, \xi'_1) \mathrm{d}\xi_1 \cdots \mathrm{d}\xi_m \mathrm{d}\xi'_k \cdots \mathrm{d}\xi'_1. \tag{5.51}$$

We can restrict (5.51) to $\Phi \in \otimes^k_{\rm s/a} \mathcal{Z}$ to $\Psi \in \otimes^m_{\rm s/a} \mathcal{Z}$. Then (5.51) will depend only on the symmetrization/antisymmetrization of b, that is

$$b^{\rm s/a} := \Theta^m_{\rm s/a} b \Theta^k_{\rm s/a}. \tag{5.52}$$

Thus to describe integral kernels of operators from $\otimes^k_{\rm s/a} \mathcal{Z}$ to $\otimes^m_{\rm s/a} \mathcal{Z}$ it is enough to consider functions symmetric/antisymmetric separately wrt the first m and the last k arguments.

In this subsection we will put "hats" on the creation/annihillation operators. The symbols $a^*(\xi)$, $a(\xi)$ without hats will be reserved for classical variables, which in the bosonic case commute and in the fermionic anticommute.

By a *polynomial on* $\overline{\mathcal{Z}} \oplus \mathcal{Z}$ we will mean a linear combination of the following expressions

$$b(a^*, a) = \int \cdots \int b(\xi_1, \cdots \xi_m, \xi'_k, \cdots, \xi'_1) \tag{5.53}$$
$$a^*(\xi_1) \cdots a^*(\xi_m) a(\xi'_k) \cdots a(\xi'_1) \mathrm{d}\xi_1 \cdots \mathrm{d}\xi_m \mathrm{d}\xi'_k \cdots \mathrm{d}\xi'_1,$$

where b are symmetric/antisymmetric separately wrt the first m and the last k arguments. In the symmetric case this can be interpreted as a usual *polynomial on* $\overline{\mathcal{Z}} \oplus \mathcal{Z}$, but it is common to use this term also in the antisymmetric case.

The *Wick quantization of* $b(a^*, a)$ is defined as

$$\begin{aligned} b(\hat{a}^*, \hat{a}) &= \int b(\xi_1, \cdots \xi_m, \xi'_k, \cdots, \xi'_1) \\ &\quad \hat{a}^*(\xi_1) \cdots \hat{a}^*(\xi_m) \hat{a}(\xi'_k) \cdots \hat{a}(\xi'_1) \mathrm{d}\xi_1, \cdots \mathrm{d}\xi_k \mathrm{d}\xi'_1 \cdots \mathrm{d}\xi'_m. \end{aligned} \tag{5.54}$$

(Actually, by (5.52), in (5.53) and (5.54) we can consider b which is not symmetric/antisymmetric.)

Here is an equivalent definition of $b(\hat{a}, \hat{a})$: Its only nonzero matrix elements are between $\Phi \in \otimes_{\mathrm{s/a}}^{p+m} \mathcal{Z}$, $\Psi \in \otimes_{\mathrm{s/a}}^{p+k} \mathcal{Z}$, and equal

$$(\Phi | b(\hat{a}^*, \hat{a}) \Psi) = \frac{\sqrt{(m+p)!(k+p)!}}{p!} (\Phi | b \otimes 1_{\mathcal{Z}}^{\otimes p} \Psi). \tag{5.55}$$

To see this it is enough to use the formal identity (5.22) several times:

$$\begin{aligned} &\big(\Phi | \hat{a}^*(\xi_1) \cdots \hat{a}^*(\xi_m) \hat{a}(\xi'_k) \cdots \hat{a}(\xi'_1) \Psi\big) && (5.56) \\ =&\big(\hat{a}(\xi_m) \cdots \hat{a}(\xi_1) \Phi | \hat{a}(\xi'_k) \cdots \hat{a}(\xi'_1) \Psi\big) && (5.57) \\ =&\sqrt{(m+p) \cdots (p+1)(k+p) \cdots (p+1)} && (5.58) \\ &\times \int \overline{\Phi(\xi_m, \ldots, \xi_1, \eta_p, \ldots, \eta_1)} \Psi(\xi'_m, \ldots, \xi'_1, \eta_p, \ldots, \eta_1) \mathrm{d}\eta_p \cdots \mathrm{d}\eta_1. && (5.59) \end{aligned}$$

Essentially every operator on a Fock space can be written as a linear combination of (5.54).

5.11 Wick symbol and coherent states

In the bosonic case, we have the identities

$$\mathrm{e}^{-\hat{a}^*(b) + \hat{a}(b)} \hat{a}(v) \mathrm{e}^{\hat{a}^*(b) - \hat{a}(b)} = \hat{a}(v) + (v|b), \tag{5.60}$$

$$\mathrm{e}^{-\hat{a}^*(b) + \hat{a}(b)} \hat{a}^*(v) \mathrm{e}^{\hat{a}^*(b) - \hat{a}(b)} = \hat{a}(v) + (v|b). \tag{5.61}$$

We also introduce the coherent state corresponding to $b \in \mathcal{Z}$:

$$\Omega_b := \mathrm{e}^{\hat{a}^*(b) - \hat{a}(b)} \Omega. \tag{5.62}$$

Note that $\hat{a}(v)\Omega_b = (v|b)\Omega_b$. We have the identity

$$(\Omega_b | c(\hat{a}^*, \hat{a}) \Omega_b) = c(b^*, b). \tag{5.63}$$

5.12 Particle number preserving operators

If $m = k$, then the operator $b(\hat{a}^*, \hat{a})$ preserves the number of particles and (5.55). For $\Phi \in \otimes^n_{\mathrm{s/a}}\mathcal{Z}$, $\Psi \in \otimes^n_{\mathrm{s/a}}\mathcal{Z}$ it can be rewritten as

$$(\Phi|b(\hat{a}^*, \hat{a})\Psi) \quad = \quad \frac{n!}{(n-m)!}(\Phi|b \otimes 1_{\mathcal{Z}}^{\otimes(n-m)}\Psi). \tag{5.64}$$

But $\frac{n!}{(n-m)!m!}$ is the number of m-element subsets of $\{1, 2, \ldots, n\}$. Therefore in the obvious notation, we can rewrite (5.64) as

$$\frac{1}{m!}b(\hat{a}^*, \hat{a}) = \sum_{1 \le i_1 < \cdots < i_m \le n} b_{i_1,\ldots,i_m}. \tag{5.65}$$

In particular, for $m = 2$ we can write

$$\frac{1}{2}b(\hat{a}^*, \hat{a}) = \sum_{1 \le i < j \le n} b_{ij}. \tag{5.66}$$

Finally, for $m = 1$, we have

$$b(\hat{a}^*, \hat{a}) = \sum_{1 \le i \le n} b_i = \mathrm{d}\Gamma(b). \tag{5.67}$$

5.13 Examples

Consider the Schrödinger Hamiltonian of n identical particles on $L^2(\mathbb{R}^{dN})$

$$H_n = -\sum_{i=1}^n \Delta_i + \sum_{1 \le i < j \le n} V(x_i - x_j), \tag{5.68}$$

$$P_n = \sum_{i=1}^n \frac{1}{\mathrm{i}}\partial_{x_i}, \tag{5.69}$$

In the momentum representation

$$\begin{aligned} H_n \quad &= \quad \sum_{i=1}^n p_i^2 \\ &\quad\quad +(2\pi)^{-d} \sum_{1 \le i < j \le N} \delta(p_i' + p_j' - p_j - p_i)\hat{V}(p_i' - p_i). \\ P_n \quad &= \quad \sum_{i=1}^n p_i. \end{aligned}$$

Consider the 2nd quantization of $L^2(\mathbb{R}^d)$. We have the position representation, with the generic variables x, y and the momentum representation with the

generic variables k, k'. We can pass from one representation to the other by

$$a^*(k) = (2\pi)^{-\frac{d}{2}} \int a^*(x) \mathrm{e}^{-\mathrm{i}kx} \mathrm{d}x, \quad a^*(x) = (2\pi)^{-\frac{d}{2}} \int a^*(k) \mathrm{e}^{\mathrm{i}kx} \mathrm{d}k, \tag{5.70}$$

$$a(k) = (2\pi)^{-\frac{d}{2}} \int a(x) \mathrm{e}^{\mathrm{i}kx} \mathrm{d}x, \qquad a(x) = (2\pi)^{-\frac{d}{2}} \int a(k) \mathrm{e}^{-\mathrm{i}kx} \mathrm{d}k. \tag{5.71}$$

In the 2nd quantized notation we can rewrite all this as

$$\begin{aligned} H := \bigoplus_{n=0}^{\infty} H_n &= -\int a_x^* \Delta_x a_x \mathrm{d}x && (5.72) \\ &\quad + \int\int \mathrm{d}x\mathrm{d}y V(x-y) a_x^* a_y^* a_y a_x \\ &= \int p^2 a_p^* a_p \mathrm{d}p && (5.73) \\ &\quad + (2\pi)^{-d} \int\int\int \mathrm{d}p\mathrm{d}q\mathrm{d}k \hat{V}(k) a_{p+k}^* a_{q-k}^* a_q a_p \\ P := \bigoplus_{n=0}^{\infty} P_n &= \int a_x^* \frac{1}{\mathrm{i}} \partial_x a_x \mathrm{d}x && (5.74) \\ &= \int p a_p^* a_p \mathrm{d}p. && (5.75) \end{aligned}$$

Consider $L^2([0,L]^d) \simeq L^2\left(\frac{2\pi}{L}\mathbb{Z}^d\right)$ and its 2nd quantization. Again we use x, y in the position representation with periodic boundary conditions and k, k' in the momentum representation. We can pass from one representation to the other by

$$a^*(k) = L^{-\frac{d}{2}} \int a(x) \mathrm{e}^{-\mathrm{i}kx} \mathrm{d}x, \qquad a^*(x) = L^{-\frac{d}{2}} \sum_k a(k) \mathrm{e}^{\mathrm{i}kx}, \tag{5.76}$$

$$a(k) = L^{-\frac{d}{2}} \int a(x) \mathrm{e}^{\mathrm{i}kx} \mathrm{d}x, \qquad a(x) = L^{-\frac{d}{2}} \sum_k a(k) \mathrm{e}^{-\mathrm{i}kx}. \tag{5.77}$$

Here are the analogs of (5.73) and (5.75):

$$\begin{aligned} H &= \sum_p p^2 a_p^* a_p \\ &\quad + L^{-d} \sum_p \sum_q \sum_k \hat{V}(k) a_{p+k}^* a_{q-k}^* a_q a_p, \\ P &= \sum_p p a_p^* a_p. \end{aligned}$$

6 Formalism of classical mechanics

6.1 Dynamical systems

Suppose that a system is described by a manifold $\mathcal{Y}$ called a "phase space". The space $C^\infty(\mathcal{Y})$ of smooth functions on $\mathcal{Y}$ describes possible observables.

To define a dynamics one needs to fix a vector field V on $\mathcal{Y}$ and one has the *equations of motion*

$$\frac{\mathrm{d}}{\mathrm{d}t}\zeta(t) = V\big(\zeta(t)\big), \quad \zeta(0) = \zeta_0. \tag{6.1}$$

The evolution of an observable $F \in C^\infty(\mathcal{Y})$ is then given by

$$\frac{\mathrm{d}}{\mathrm{d}t}F(\zeta) = \langle \mathrm{d}F(\zeta) | V(\zeta) \rangle. \tag{6.2}$$

Let us fix coordinates y^i on $\mathcal{Y}$, that is functions $\mathcal{Y} \ni \zeta \mapsto y^i(\zeta) \in \mathbb{R}$. Then for each $\zeta \in \mathcal{Y}$, the tangent space $\mathrm{T}_\zeta\mathcal{Y}$ is spanned by the vectors $\frac{\partial}{\partial y^i}$ and its dual, called the cotangent space, by the 1-forms $\mathrm{d}y^i$. They satisfy

$$\Big\langle \mathrm{d}y^i | \frac{\partial}{\partial y^j} \Big\rangle = \delta^j_i. \tag{6.3}$$

The vector field V can be written as $V(\zeta) = V^i(\zeta)\frac{\partial}{\partial y^i}$ and the 1-form $\mathrm{d}F$ as $\mathrm{d}F(\zeta) = \frac{\partial F(\zeta)}{\partial y^i}\mathrm{d}y^i$, and the equations (6.1) and (6.2) become

$$\frac{\mathrm{d}}{\mathrm{d}t}y^i(\zeta(t)) = V^i\big(\zeta(t)\big), \tag{6.4}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}F(\zeta) = \frac{\partial F(\zeta)}{\partial y^i} \cdot V^i(\zeta). \tag{6.5}$$

6.2 Hamiltonian dynamics

Let us first recall basic facts about Hamiltonian dynamics. Let us begin with the phase space $\mathcal{Y} = \mathbb{R}^{2n}$ with coordinates ϕ^i, π_j, $i = 1, \ldots, n$. (This choice of symbols anticipates our main modivation: field theory). Let us consider a *Hamiltonian* H, that is a function on the phase space, so that it can be expressed in terms of ϕ and π. The *Hamilton equations* generated by H are

$$\frac{\mathrm{d}}{\mathrm{d}t}(\phi^i, \pi_i) = \big(\partial_{\pi_i}H(\phi,\pi), -\partial_{\phi^i}H(\phi,\pi)\big)\,. \tag{6.6}$$

Another form:

$$\frac{\mathrm{d}}{\mathrm{d}t}\begin{bmatrix}\phi\\ \pi\end{bmatrix} = \begin{bmatrix}0 & 1\\ -1 & 0\end{bmatrix}\begin{bmatrix}\partial_\phi H\\ \partial_\pi H\end{bmatrix}. \tag{6.7}$$

A vector field of the form

$$\partial_{\pi_i}H(\phi,\pi)\frac{\partial}{\partial\phi^i} - \partial_{\phi^i}H(\phi,\pi)\frac{\partial}{\partial\pi_i} \tag{6.8}$$

for some function H is called a *Hamiltonian vector field.* Thus the Hamilton equations are given by a Hamiltonian vector field.

Given two functions F, G on $\mathcal{Y}$ one introduces the Poisson bracket which is a bilinear antisymmetric map $C^\infty(\mathcal{Y}) \times C^\infty(\mathcal{Y}) \to C^\infty(\mathcal{Y})$, as

$$\{F, G\} = \partial_{\phi^i}F\partial_{\pi_i}G - \partial_{\pi_i}F\partial_{\phi^i}G. \tag{6.9}$$

The Poisson bracket satisfies the Leibniz and Jacobi identity

$$\{F, GH\} = \{F, G\}H + G\{F, H\}, \tag{6.10}$$

$$\{\{F, G\}, H\} + \{\{G, H\}, F\} + \{\{H, F\}, G\} = 0. \tag{6.11}$$

The coordinates ϕ, π satisfy

$$\{\phi^i, \phi^j\} = \{\pi_i, \pi_j\} = 0, \quad \{\phi^i, \pi_j\} = \delta^i_j. \tag{6.12}$$

The Hamilton equations can be rewritten as

$$\frac{\mathrm{d}}{\mathrm{d}t}\phi^i = \{\phi^i, H\}, \tag{6.13}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\pi_i = \{\pi_i, H\}. \tag{6.14}$$

More generally, the evolution of every observable F is given by

$$\frac{\mathrm{d}}{\mathrm{d}t}F = \{F, H\}. \tag{6.15}$$

Note that the Poisson bracket is preserved by a Hamiltonian flow. This follows from the Jacobi identity:

$$\frac{\mathrm{d}}{\mathrm{d}t}\{F, G\} = \{\{F, H\}, G\} + \{F, \{G, H\}\} = \{\{F, G\}, H\}. \tag{6.16}$$

6.3 Symplectic form

Let us continue with the phase space $\mathcal{Y} = \mathbb{R}^{2n}$ with the coordinates ϕ^i and π_i. For any $\zeta \in \mathcal{Y}$, the tangent space $\mathrm{T}_\zeta\mathbb{R}^{2n}$ is spanned by the vectors $\frac{\partial}{\partial\phi^i}$, $\frac{\partial}{\partial\pi_i}$ and the cotangent space $\mathrm{T}^*_\zeta\mathbb{R}^{2n}$ by the 1-forms $\mathrm{d}\phi^i$, $\mathrm{d}\pi_i$. One can introduce the 2-form on $\mathcal{Y}$:

$$\omega = \mathrm{d}\pi^i \wedge \mathrm{d}\phi_i, \tag{6.17}$$

called the *symplectic form*.

Clearly,

$$\Big\langle \omega | \frac{\partial}{\partial\phi^i}, \frac{\partial}{\partial\phi^j} \Big\rangle = \Big\langle \omega | \frac{\partial}{\partial\pi_i}, \frac{\partial}{\partial\pi_j} \Big\rangle = 0, \tag{6.18}$$

$$\Big\langle \omega | \frac{\partial}{\partial\pi_i}, \frac{\partial}{\partial\phi^j} \Big\rangle = -\Big\langle \omega | \frac{\partial}{\partial\phi^i}, \frac{\partial}{\partial\pi_j} \Big\rangle = \delta^i_j. \tag{6.19}$$

One can introduce a linear map $\boldsymbol{\omega}(\zeta) : \mathrm{T}_\zeta\mathbb{R}^{2n} \to \mathrm{T}^*_\zeta\mathbb{R}^{2n}$ such that

$$\langle \omega | v, z \rangle = \langle v | \boldsymbol{\omega} z \rangle. \tag{6.20}$$

Thus

$$\boldsymbol{\omega}\Big(\frac{\partial}{\partial\phi^i}\Big) = \mathrm{d}\pi_i, \tag{6.21}$$

$$\boldsymbol{\omega}\Big(\frac{\partial}{\partial\pi_i}\Big) = -\,\mathrm{d}\phi^i. \tag{6.22}$$

Thus $\boldsymbol{\omega}$ is given by the matrix $\boldsymbol{\omega} = \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix}$. Clearly, $\boldsymbol{\omega}^{-1} = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}$. A vector field on a symplectic manifold is called Hamiltonian if it has the form

$$V(\zeta) = -\boldsymbol{\omega}^{-1}(\zeta)\mathrm{d}H(\zeta). \tag{6.23}$$

Let us note the following properties of the symplectic form:

1. $\omega(\zeta)$ is nondegenerate at every point $\zeta \in \mathcal{Y}$;
2. $\mathrm{d}\omega = 0$.

Nondegenerate means that the nullspace of $\boldsymbol{\omega}(\zeta)$ is always trivial.

One can be more general: Let $\mathcal{Y}$ be a manifold equipped with a 2-form satisfying 1. and 2. Then we say that $(\mathcal{Y}, \omega)$ is a symplectic manifold.

The Darboux Theorem says that on any symplectic manifold locally we can always choose coordinates, say ϕ^i, π_j, $i = 1, \dots, n$, such that (6.17) holds.

Specifying a symplectic form is equivalent to specifying a Poisson bracket. Indeed, we can write the Poisson bracket as

$$\{F, G\} = \langle \mathrm{d}F | \boldsymbol{\omega}^{-1} \mathrm{d}G \rangle = -\Big\langle \omega | \boldsymbol{\omega}^{-1}(\mathrm{d}F), \boldsymbol{\omega}^{-1}(\mathrm{d}G) \Big\rangle, \quad F, G \in C^\infty(\mathcal{Y}). \tag{6.24}$$

One says that a diffeomorphism $T : \mathcal{Y} \to \mathcal{Y}$ is symplectic if it preserves the symplectioc form. Equivalently, it preserves the Poisson bracket. Every flow generated by a Hamiltonian flow is symplectic.

In most our applications, the phase space wil have the structure of a vector space and ϕ^i, π_j, $i = 1, \dots, n$, can be chosen to be the coordinates in a basis. Then the tangent space to $\mathrm{T}_\zeta\mathcal{Y}$ at any point $\zeta \in \mathcal{Y}$ can be identified with $\mathcal{Y}$ itself and the form ω is simply a nondegenerate antisymmetric bilinear form on $\mathcal{Y}$. The Darboux Theorem says that we can identify a symplectic manifold with a symplectic vector space at least locally.

The space $\mathcal{Y}^{\mathrm{T}}$ of linear functionals on $\mathcal{Y}$ obviously is contained in $C^\infty(\mathcal{Y})$. For a linear functional on $\mathcal{Y}$, its derivative is the original functional itself. Therefore, (6.17) can be simplified and written as

$$\omega = \pi^i \wedge \phi_i, \tag{6.25}$$

6.4 Lagrangian formalism

Suppose that $\mathbb{R}^n$ is described by the coordinates ϕ^i. Let $L(t, \phi, \dot{\phi})$ be a function on $\mathbb{R} \times \mathbb{R}^n \times \mathbb{R}^n$ called the Lagrangian. The Euler-Lagrange equations are

$$\frac{\partial L}{\partial \phi^i} = \frac{\mathrm{d}}{\mathrm{d}t} \frac{\partial L}{\partial \dot{\phi}^i}. \tag{6.26}$$

Define the *canonical momentum conjugate to* ϕ^i, that is $\pi_i := \frac{\partial L}{\partial \dot{\phi}^i}$.

The initial consitions for (6.26) can be expressed in terms $\phi, \dot{\phi}$. Suppose that we can express $\dot{\phi}$ in terms of ϕ, π. Then initial conditions can be described in

terms of ϕ, π and we can pass from the Lagrangian to the Hamiltonian formalism. More precisely, we can introduce

$$\text{the } \textit{tautological 1-form}, \quad \theta := \pi_i \mathrm{d}\phi^i, \tag{6.27}$$

$$\text{the symplectic 2-form} \quad \omega := \mathrm{d}\pi_i \wedge \mathrm{d}\phi^i = \mathrm{d}\theta, \tag{6.28}$$

$$\text{and the Hamiltonian} \quad H(t,\phi,\pi) := \pi_i \dot{\phi}^i - L\big(t,\phi,\dot{\phi}(\phi,\pi)\big). \tag{6.29}$$

We check that $\partial_\phi H = -\partial_\phi L$, $\partial_\pi H = \dot{\phi}$. Hence the Euler-Lagrange equations imply the Hamilton equations.

6.5 Noether Theorem

Suppose that ϕ depend on a parameter α. Define

$$P := \frac{\partial L}{\partial \dot{\phi}^i} \partial_\alpha \phi^i. \tag{6.30}$$

Suppose that $L\big(t,\phi(\alpha),\dot{\phi}(\alpha)\big)$ is independent of α. The Noether Theorem says that along the evolution $P\big(t,\phi(t),\dot{\phi}(t)\big)$ is constant. Indeed,

$$\frac{\mathrm{d}}{\mathrm{d}t} P = \Big(\frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial L}{\partial \dot{\phi}^i}\Big)\phi^i_{,\alpha} + \frac{\partial L}{\partial \dot{\phi}^i}\frac{\mathrm{d}}{\mathrm{d}t}\phi^i_{,\alpha} \tag{6.31}$$

$$= \frac{\partial L}{\partial \phi^i}\phi^i_{,\alpha} + \frac{\partial L}{\partial \dot{\phi}^i}\dot{\phi}^i_{,\alpha} = \frac{\mathrm{d}L}{\mathrm{d}\alpha} = 0. \tag{6.32}$$

If $\alpha = \vec{x}$, so that the Lagrangian is invariant wrt translations, then P is called the *(total) momentum*. (Note a confusing collision of terminology with *canonical momenta*).

6.6 Classical field theory–Lagrangian formalism

Consider the space $\mathbb{R}^d$ (the "spacetime", where however the metric or Lorentz structure is for the moment irrelevant) and a space $\mathbb{R}^n$ (the "internal degrees of freedom", whose indices will be as a rule omitted). A *field configuration* is a function $\mathbb{R}^d \ni x \mapsto \zeta(x) = [\zeta^i(x)] \in \mathbb{R}^n$. The *classical field* $\phi^i(x)$ is the "value of the ith coordinate at x of the field configuration", that is

$$\langle \phi^i(x) | \zeta \rangle = \zeta^i(x). \tag{6.33}$$

Thus the classical field is a linear functional on field configurations.

Suppose that $\mathcal{L}(x) = \mathcal{L}(x, \phi(x), \phi_{,\mu}(x))$ is a function called the *Lagrangian density*.

$$I := \int \mathcal{L}(x) \mathrm{d}x \tag{6.34}$$

is called the *action*. Thus the action is a (typically nonlinear) functional on field configurations.

Let us compute the the derivative in the direction of $\varepsilon \in C_{\mathrm{c}}^{\infty}(\mathbb{R}^d)$ of the action at the configuration ζ:

$$\begin{aligned}
&\langle I|\zeta+\varepsilon\rangle - \langle I|\zeta\rangle \\
&= \int \Big(\mathcal{L}\big(x,\zeta(x)+\varepsilon(x),\zeta_{,\mu}(x)+\varepsilon_{,\mu}(x)\big) - \mathcal{L}\big(x,\zeta(x),\zeta_{,\mu}(x)\big)\Big)\mathrm{d}x \\
&\approx \int \frac{\partial \mathcal{L}}{\partial \phi(x)}(x,\zeta(x),\zeta_{,\mu}(x))\varepsilon(x)\mathrm{d}x + \int \frac{\partial \mathcal{L}}{\partial \phi_{,\mu}(x)}(x,\zeta(x),\zeta_{,\mu}(x))\varepsilon_{,\mu}(x)\mathrm{d}x \\
&= \int \Big(\frac{\partial \mathcal{L}}{\partial \phi(x)}(x,\zeta(x),\zeta_{,\mu}(x)) - \partial_\mu \frac{\partial \mathcal{L}}{\partial \phi_{,\mu}(x)}(x,\zeta(x),\zeta_{,\mu}(x))\Big)\varepsilon(x)\mathrm{d}x \qquad (6.35)\\
&\quad + \int \partial_\mu\Big(\frac{\partial \mathcal{L}}{\partial \phi_{,\mu}(x)}(x,\zeta(x),\zeta_{,\mu}(x))\varepsilon(x)\Big)\mathrm{d}x
\end{aligned}$$

The last term vanishes by the Stokes Theorem. Hence the derivative in the direction of ε is given by (6.35). If we require that ζ is a stationary point for the action, that is, this derivative vanishes, we obtain the Euler-Lagrange equations:

$$\partial_{\phi(x)}\mathcal{L}(x) - \partial_\mu \frac{\partial \mathcal{L}(x)}{\partial \phi_{,\mu}(x)} = 0 \qquad (6.36)$$

Let $\pi^\mu(x)$ denote the *canonical momentum conjugate to* $\phi(x)$ *in the direction of* x^μ:

$$\pi^\mu(x) = \frac{\partial \mathcal{L}(x)}{\partial \phi_{,\mu}(x)}. \qquad (6.37)$$

Consider the space of solutions of the Euler-Lagrange equations. The operation d will denote the exterior derivative on this (infinite dimensional) space. Similarly, on this space we use $\wedge$. If something holds on solutions of the Euler-Lagrange equation, we will say that it is true *on shell*.

We introduce

$$\text{the } \textit{tautological current} \quad \theta^\mu(x) := \pi^\mu(x)\mathrm{d}\phi(x), \qquad (6.38)$$

$$\text{the } \textit{symplectic current} \quad j^\mu(x) := \mathrm{d}\pi^\mu(x) \wedge \mathrm{d}\phi(x) = \mathrm{d}\theta^\mu. \qquad (6.39)$$

On shell the divergence of the tautological current is the differential of the Lagrangian and that of the symplectic current vanishes:

$$\partial_\mu \theta^\mu(x) = \mathrm{d}\mathcal{L}, \qquad (6.40)$$

$$\partial_\mu j^\mu(x) = 0. \qquad (6.41)$$

Indeed,

$$\begin{aligned}
\partial_\mu \theta^\mu(x) &= \partial_\mu \frac{\partial \mathcal{L}(x)}{\partial \phi_{,\mu}(x)}\mathrm{d}\phi(x) + \frac{\partial \mathcal{L}(x)}{\partial \phi_{,\mu}(x)}\mathrm{d}\phi_{,\mu}(x) \qquad (6.42)\\
&= \frac{\partial \mathcal{L}(x)}{\partial \phi(x)}\mathrm{d}\phi(x) + \frac{\partial \mathcal{L}(x)}{\partial \phi_{,\mu}(x)}\mathrm{d}\phi_{,\mu}(x) = \mathrm{d}\mathcal{L}(x). \qquad (6.43)\\
\partial_\mu j^\mu(x) &= \partial_\mu \mathrm{d}\theta^\mu(x) = \mathrm{d}\partial_\mu \theta^\mu(x) = \mathrm{d}\mathrm{d}\mathcal{L}(x) = 0. \qquad (6.44)
\end{aligned}$$

Introduce the *Noetherian stress-energy tensor*

$$\mathcal{T}^{\mu}_{\nu}(x) \quad := \quad -\frac{\partial \mathcal{L}(x)}{\partial \phi_{,\mu}(x)}\phi_{,\nu}(x) + \delta^{\mu}_{\nu}\mathcal{L}(x). \tag{6.45}$$

Here is the Noether Theorem in the context of classical field theory: on shell we have

$$\partial_{\mu}\mathcal{T}^{\mu}_{\nu}(x) = \partial_{\nu}\mathcal{L}(x) \tag{6.46}$$

In particular, if $\mathcal{L}$ is invariant wrt translations, then the stress-energy tensor is conserved (its divergence vanishes).

Indeed,

$$\partial_{\mu}\mathcal{T}^{\mu}_{\nu}(x) = -\partial_{\mu}\Big(\frac{\partial \mathcal{L}(x)}{\partial \phi_{,\mu}(x)}\Big)\phi_{,\nu}(x) - \frac{\partial \mathcal{L}(x)}{\partial \phi_{,\mu}(x)}\phi_{,\mu\nu}(x) \tag{6.47}$$

$$+ \frac{\partial \mathcal{L}(x)}{\partial \phi(x)}\phi_{,\nu}(x) + \frac{\partial \mathcal{L}(x)}{\partial \phi_{,\alpha}(x)}\phi_{,\alpha\nu}(x) + \partial_{\nu}\mathcal{L}(x). \tag{6.48}$$

Then we use the Euler-Lagrange equations (6.36).

6.7 Hyperbolic classical field theory

Suppose now that the Euler-Lagrange equations (6.36) are characterized by a finite speed of propagation. A typical example of such a situation is when $\mathbb{R}^d$ is the Minkowski space, the Lagrangian is

$$\mathcal{L}(x) = -|g|^{\frac{1}{2}}\Big(\frac{1}{2}g^{\mu\nu}\partial_{\mu}\phi(x)\partial_{\nu}\phi(x) + P(\phi(x))\Big), \tag{6.49}$$

which leads to the Klein-Gordon equation with possibly nonlinear terms:

$$-\Box_g\phi(x) = P'(\phi(x)). \tag{6.50}$$

If $P(\phi) = \frac{m^2}{2}\phi(x)^2$, then we get the linear Klein-Gordon equation

$$(-\Box_g + m^2)\phi(x) = 0. \tag{6.51}$$

One can then introduce an identification $M \simeq \mathbb{R} \times \Sigma$, where $\mathbb{R}$ describes "time" and Σ is a "spatial cross-section", in the case of the Minkowski space $\Sigma = \mathbb{R}^{d-1}$. The Lagrangian is given by the integral of the Lagrangian density over a *constant time surface* $\{t\} \times \Sigma$

$$L(t) := \int \mathcal{L}(t, \vec{x})\mathrm{d}\vec{x}. \tag{6.52}$$

The momentum conjugate to the field $\phi(t, \vec{x})$ coincides with the temporal coordinate of (6.37):

$$\pi(t, \vec{x}) := \frac{\partial L(t)}{\partial \dot{\phi}(t, \vec{x})} = \pi^0(t, \vec{x}). \tag{6.53}$$

It is natural to use the set of space-compact solutions of the Euler-Lagrange equations as the phase space. It is equipped with a symplectic form

$$\omega := \int j^0(t,\vec{x})\mathrm{d}\vec{x} = \int \mathrm{d}\pi^0(t,\vec{x}) \wedge \mathrm{d}\phi(t,\vec{x})\mathrm{d}\vec{x}. \tag{6.54}$$

Using (6.41) we can show that (6.54) does not depend on t. Actually, instead of integrating over $\{t\} \times \Sigma$, we can integrate the symplectic current over any "Cauchy surface" obtaining the same ω.

The symplectic form ω corresponds to the equal-time Poisson brackets

$$\begin{aligned} \{\phi(t,\vec{x}),\phi(t,\vec{y})\} = \{\pi(t,\vec{x}),\pi(t,\vec{y})\} &= 0, \\ \{\phi(t,\vec{x}),\pi(t,\vec{y})\} &= \delta(\vec{x}-\vec{y}). \end{aligned} \tag{6.55}$$

Let us call minus the 00-component of the stress-energy tensor the Hamiltonian density:

$$\mathcal{H}(x) := -\mathcal{T}^0_0(x) = \pi(x)\dot{\phi}(x) - \mathcal{L}(x). \tag{6.56}$$

The Hamiltonian obtained from the Lagrangian by the Legendre transformation coincides with the integral of the Hamiltonian density over the corresponding constant time surface:

$$H(t) := \int \dot{\phi}(t,\vec{x})\pi(t,\vec{x})\mathrm{d}\vec{x} - L(t) = \int \mathcal{H}(t,\vec{x})\mathrm{d}\vec{x}. \tag{6.57}$$

7 Canonical Commutation Relations

The main purpose of this section is to describe quantization in its most elementary context: that of symplectic vector spaces. Some of its material overlaps with the previous section.

7.1 Symplectic vector spaces

Let $\mathcal{Y}$ be a vector space. Recall that it is called symplectic if it is equipped with a nondegenerate antisymmetric 2-form. Thus we have a bilinear form

$$\mathcal{Y} \times \mathcal{Y} \ni (y,z) \mapsto \omega(y,z) \tag{7.1}$$

such that $\omega(y,z) = -\omega(z,y)$ and for every $y \neq 0$ we can find z such that $\omega(y,z) \neq 0$.

Clearly, every symplectic vector space is a symplectic manifold, so one can use terminology from the previous section. However, in this section the emphasis not on classical mechanics, but on is quantum mechanics, and quantization of symplectic manifolds is somewhat problematic, unlike quantization of symplectic vector spaces.

Every finite dimensional symplectic vector space has even dimension. If we choose a basis, we can write

$$\omega(y,z)=\sum_{ij}\omega_{ij}y^iz^j,\quad y=(y^i),w=(w^i)\in\mathcal{Y},\tag{7.2}$$

where $[\omega_{ij}]$ is an antisymmetric invertible matrix.

In this section we will also use slightly different notation than in the previous sectin. The notation will be adapted to quantum mechanics. Let ϕ^i, $i=1,\dots,2n$, denote the coordinate functionals, that is for $y\in\mathcal{Y}$ we have $\phi^i(y)=y^i$. Then using

$$\phi^i\wedge\phi^j(y,z)=\phi^i(y)\phi^j(z)-\phi^i(z)\phi^j(y).\tag{7.3}$$

we see that (7.2) can be written as $\omega=\frac{1}{2}\omega_{ij}\phi^i\wedge\phi^j$.

Let $[\omega^{ij}]$ be the inverse of $[\omega_{ij}]$. Then it is also an invertible antisymmetric matrix. We can equip functions on $\mathcal{Y}$ with a Poisson bracket: for $F,G\in C^\infty(\mathcal{Y})$ we set

$$\{F,G\}=-\sum\omega^{ij}\partial_{\phi^i}F\partial_{\phi^j}G.\tag{7.4}$$

In particular,

$$\{\phi^i,\phi^j\}=-\omega^{ij}.\tag{7.5}$$

We say that a symplectic space is $\mathbb{R}^{2n}$ is equipped with a *symplectic basis* if the symplectic form is given by the matrix

$$\omega=\begin{bmatrix}0&\mathbb{1}\\-\mathbb{1}&0\end{bmatrix}.\tag{7.6}$$

In every finite dimensional symplectic vector space we can find a symplectic basis. It is then natural to separate the variables into two families, writing $x^i=\phi^i$, $p_i:=\phi^{n+i}$, $i=1,\dots,n$. Then $\omega=x^i\wedge p_i$ and

$$\{F,G\}=\partial_{x^i}F\partial_{p_i}G-\partial_{p_i}F\partial_{x^i}G.\tag{7.7}$$

In particular,

$$\{x^i,x^j\}=\{p_i,p_j\}=0,\quad\{x^i,p_j\}=\delta^i_j.\tag{7.8}$$

Recall that by an affine transformation on a vector space $\mathcal{Y}$ we mean a transformation of the form

$$\mathcal{Y}\ni y\mapsto Ty+z\in\mathcal{Y},\tag{7.9}$$

where T is linear and $z\in\mathcal{Y}$.

A linear transformation T on a symplectic space $(\mathcal{Y},\omega)$ is called symplectic if it preserves the symplectic form, that is

$$\omega(Ty,Tz)=\omega(y,z).\tag{7.10}$$

We say that an affine transformation (7.9) is symplectic, if T is symplectic. Note that this terminology is consistent with the one introduced for symplectic manifolds.

Equivalently, an affine transformation is symplectic if it preserves the Poisson product: that means

$$\{F \circ T, G \circ T\} = \{F, G\} \circ T, \tag{7.11}$$

where $\circ$ denotes the composition.

7.2 Quantization of linear and quadratic observables

Let $(\mathcal{Y}, \omega)$ be a symplectic space. Informally one can say that quantization is a map that to a function F on $\mathcal{Y}$ associates an operator $\hat{F}$ on a certain Hilbert space $\mathcal{H}$, which satisfies the following conditions:

$$\hat{1} = \mathbb{1}; \tag{7.12}$$

$$\frac{1}{2}(\hat{F}\hat{G} + \hat{G}\hat{F}) \approx \widehat{FG}; \tag{7.13}$$

$$[\hat{F}, \hat{G}] \approx \mathrm{i}\hbar\widehat{\{F, G\}}. \tag{7.14}$$

Here $\hbar$ is a small positive parameter and $\approx$ means some kind of equality modulo terms small for small $\hbar$.

One can prove that one cannot replace $\approx$ with $=$.

As we discussed above, if $\mathcal{Y}$ is finite dimensional, we can always find coordinates x^i, p_i, $i = 1, \dots, n$ satisfying (7.8). In other words, $\mathcal{Y} = \mathbb{R}^{2n} = \mathbb{R}^n \oplus \mathbb{R}^n$ is a symplectic vector space equipped with a symplectic basis.

With the above classical system we associate a quantum system as follows. Let $\hbar$ be a real parameter. We consider the Hilbert space $\mathcal{H} := L^2(\mathbb{R}^n)$ equipped with the operators

$$\hat{x}^i \Psi(x) = x^i \Psi(x), \qquad \hat{p}_i \Psi(x) := \hbar \frac{\partial}{\mathrm{i}\partial x^i} \Psi(x). \tag{7.15}$$

They satisfy the *Heisenberg commutation relations*:

$$[\hat{x}^i, \hat{x}^j] = [\hat{p}_i, \hat{p}_j] = 0, \quad [\hat{x}^i, \hat{p}_j] = \mathrm{i}\hbar\delta^i_j. \tag{7.16}$$

Note that 1st degree polynomials, that is,

$$V = \xi_i x^i + \eta^i p_i + c, \tag{7.17}$$

$$\hat{V} = \xi_i \hat{x}^i + \eta^i \hat{p}_i + c\mathbb{1}. \tag{7.18}$$

satisfy (7.14) exactly:

$$[\hat{V}, \hat{V}'] = \mathrm{i}\hbar\widehat{\{V, V'\}} \tag{7.19}$$

One would like to extend the quantization to more general functions, not only 1st order polynomials. There are many possibilities in the literature (e.g. the Weyl quantization, Wick quantization, etc.). We will not discuss them here.

Actually, for our present purposes we will only need quantization of second order polynomials, which we define as follows:

$$H = \frac{1}{2}A_{ij}x^i x^j + \frac{1}{2}B^{ij}p_i p_j + C_i^j x^i p_j, \tag{7.20}$$

$$\hat{H} = \frac{1}{2}A_{ij}\hat{x}^i\hat{x}^j + \frac{1}{2}B^{ij}\hat{p}_i\hat{p}_j + \frac{1}{2}C_i^j(\hat{x}^i\hat{p}_j + \hat{p}_j\hat{x}^i). \tag{7.21}$$

Note that with this definition we have exact versions of (7.13) and (7.14)

$$[\hat{H}, \hat{H}'] = \mathrm{i}\hbar\widehat{\{H, H'\}}, \tag{7.22}$$

$$\frac{1}{2}(\hat{V}\hat{V}' + \hat{V}'\hat{V}) = \widehat{VV'} \tag{7.23}$$

for polynomials V, V' of degree ≤ 1 and for polynomials H, H' of degree ≤ 2.

7.3 Quantization of symplectic transformations

Let H be a Hamiltonian given by a quadratic polynomial on a symplectic vector space $\mathcal{Y}$ with the coordinates ϕ^i, $i = 1, \ldots, 2n$.

$$H = \frac{1}{2}\sum h_{ij}\phi^i\phi^j + \sum_i d_i\phi^i. \tag{7.24}$$

The Hamilton equations

$$\frac{\mathrm{d}}{\mathrm{d}t}\phi^i(t) = \{\phi^i(t), H\}, \tag{7.25}$$

define an affine symplectic transformation

$$\phi(0) \mapsto \phi(t). \tag{7.26}$$

Note that if the variables are divided into "positions" and "momenta", then in general they are mixed by the flow generated by a quadratic Hamiltonian. What is preserved is the "symplectic structure".

The variables $\phi(t)$ are 1st order polynomials and we can quantize them obtaining $\widehat{\phi(t)}$. Likewise, we can quantize H obtaining $\hat{H}$.

Theorem 7.1.

$$\widehat{\phi^i(t)} = \mathrm{e}^{\mathrm{i}t\frac{\hat{H}}{\hbar}}\widehat{\phi^i(0)}\mathrm{e}^{-\mathrm{i}t\frac{\hat{H}}{\hbar}}. \tag{7.27}$$

Proof. Clearly, (7.27) is satisfied for $t = 0$. We check that $\widehat{\phi(t)}$ satisfies the Heisenberg equations:

$$\mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t}\widehat{\phi^i(t)} = \mathrm{i}\hbar\widehat{\{\phi(t), H\}} = [\widehat{\phi^i(t)}, \hat{H}], \tag{7.28}$$

This implies (7.27) for all t. □

Thus we can first solve the classical Hamilton equations obtaining $\phi(t)$ and then put the hat, or first put the hat and then solve the quantum Heisenberg equation—we obtain the same $\hat{\phi}(t)$.

7.4 Weyl operators

Proposition 7.2 (Baker-Campbell-Hausdorff formula)**.** *Suppose that*

$$\big[[A,B],A\big] = \big[[A,B],B\big] = 0.$$

Then

$$\mathrm{e}^{A+B} = \mathrm{e}^{A}\mathrm{e}^{B}\mathrm{e}^{-\frac{1}{2}[A,B]}.$$

Proof. We will show that for any $t \in \mathbb{R}$

$$\mathrm{e}^{t(A+B)} = \mathrm{e}^{tA}\mathrm{e}^{tB}\mathrm{e}^{-\frac{1}{2}t^2[A,B]}. \tag{7.29}$$

First, using the Lie formula, we obtain

$$\begin{aligned} \mathrm{e}^{tA}B\mathrm{e}^{-tA} &= \sum_{n=0}^{\infty}\frac{t^n}{n!}\mathrm{ad}_A^n(B) \\ &= B + t[A,B]. \end{aligned}$$

Now

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t}\mathrm{e}^{tA}\mathrm{e}^{tB}\mathrm{e}^{-\frac{1}{2}t^2[A,B]} &= A\mathrm{e}^{tA}\mathrm{e}^{tB}\mathrm{e}^{-\frac{1}{2}t^2[A,B]} \\ &\quad +\mathrm{e}^{tA}B\mathrm{e}^{tB}\mathrm{e}^{-\frac{1}{2}t^2[A,B]} \\ &\quad -\mathrm{e}^{tA}\mathrm{e}^{tB}t[A,B]\mathrm{e}^{-\frac{1}{2}t^2[A,B]} \\ &= (A+B)\mathrm{e}^{tA}\mathrm{e}^{tB}\mathrm{e}^{-\frac{1}{2}t^2[A,B]}. \end{aligned}$$

Besides, (7.29) is true for $t = 1$. □

Let $\xi = (\xi_1, \ldots, \xi_d)$, $\eta = (\eta^1, \ldots, \eta^d) \in \mathbb{R}^d$. We will write

$$\hat{x}(\xi) := \xi_i \hat{x}^i, \quad \hat{p}(\eta) := \eta^j \hat{p}_j.$$

Clearly,

$$[\hat{x}(\xi), \hat{p}(\eta)] = \mathrm{i}\hbar\xi\cdot\eta.$$

Therefore,

$$\begin{aligned} \mathrm{e}^{\mathrm{i}\hat{x}(\xi)}\mathrm{e}^{\mathrm{i}\hat{p}(\eta)} &= \mathrm{e}^{-\frac{\mathrm{i}\hbar}{2}\xi\eta}\mathrm{e}^{\mathrm{i}(\hat{x}(\xi)+\hat{p}(\eta))} && (7.30) \\ &= \mathrm{e}^{-\mathrm{i}\hbar\xi}\mathrm{e}^{\mathrm{i}\hat{p}(\eta)}\mathrm{e}^{\mathrm{i}\hat{x}(\xi)}. && (7.31) \end{aligned}$$

The operators $\mathrm{e}^{\mathrm{i}(\hat{x}(\xi)+\hat{p}(\eta))}$ are sometimes called *Weyl operators*. They satisfy the *Weyl commutation relations*:

$$\mathrm{e}^{\mathrm{i}(\hat{x}(\xi)+\hat{p}(\eta))}\mathrm{e}^{\mathrm{i}(\hat{x}(\xi')+\hat{p}(\eta'))} = \mathrm{e}^{-\frac{\mathrm{i}\hbar}{2}(\xi\eta'-\eta\xi')}\mathrm{e}^{\mathrm{i}\left(\hat{x}(\xi+\xi')+\hat{p}(\eta+\eta')\right)}. \tag{7.32}$$

The Weyl commutation relations, at least formally, imply the Heisenberg commutation relations.

Weyl operators translate the position and momentum:

$$\begin{aligned} \mathrm{e}^{\frac{\mathrm{i}}{\hbar}(-\hat{p}(y)+\hat{x}(w))}\hat{x}\mathrm{e}^{\frac{\mathrm{i}}{\hbar}(\hat{p}(y)-\hat{x}(w))} &= \hat{x} - y, \\ \mathrm{e}^{\frac{\mathrm{i}}{\hbar}(-\hat{p}(y)+\hat{x}(w))}\hat{p}\mathrm{e}^{\frac{\mathrm{i}}{\hbar}(\hat{p}(y)-\hat{x}(w))} &= \hat{p} - w. \end{aligned}$$

7.5 Stone-von Neumann Theorem

Operators $\hat{x}^i$, $\hat{p}_i$ are unbounded. Hence the Heisenberg commutation relations (7.16) are problematic–without specifying the domain it is not clear what they precisely mean. The Weyl commutation relations (7.32) involve only bounded operators, hence their meaning is clear.

The following theorem is one of mathematical foundations of Quantum Mechanics:

Theorem 7.3. *Suppose that*

$$\mathbb{R}^{2n} \ni (\xi, \eta) \mapsto \hat{W}(\xi, \eta) \in U(\mathcal{H}) \tag{7.33}$$

is a family of operators satisfying

1. the Weyl commutation relations:

$$\hat{W}(\xi, \eta)\hat{W}(\xi', \eta') = \mathrm{e}^{-\frac{\mathrm{i}\hbar}{2}(\xi\eta' - \eta\xi')}\hat{W}(\xi + \xi', \eta + \eta'),$$

2. strong continuity: $\mathbb{R}^{2n} \ni (\xi, \eta) \mapsto \hat{W}(\xi, \eta)\Psi$ *is continuous,*

3. irreducibility: *there are no nontrivial subspaces in* $\mathcal{H}$ *invariant wrt* $\hat{W}(\xi, \eta)$.

Then there exists a unitary $U : \mathcal{H} \to L^2(\mathbb{R}^n)$ *such that*

$$U\hat{W}(\xi, \eta)U^* = \mathrm{e}^{\mathrm{i}(\hat{x}(\xi) + \hat{p}(\eta))}. \tag{7.34}$$

If we drop the irreducibility condition, then there exists a Hilbert space $\mathcal{K}$ *and a unitary operator* $U : \mathcal{H} \to L^2(\mathbb{R}^n) \otimes \mathcal{K}$ *such that*

$$U\hat{W}(\xi, \eta)U^* = \mathrm{e}^{\mathrm{i}(\hat{x}(\xi) + \hat{p}(\eta))} \otimes \mathcal{K}. \tag{7.35}$$

7.6 Representations of the CCR

Let $(\mathcal{Y}, \omega)$ be a symplectic space, possibly infinite dimensional. Let $\mathcal{H}$ be a Hilbert space. We say that a map

$$\mathcal{Y} \ni y \mapsto \hat{W}(y) \in U(\mathcal{H}) \tag{7.36}$$

is a *representation of the CCR* or a *CCR representation* if

$$\hat{W}(y)\hat{W}(y') = \mathrm{e}^{-\frac{\mathrm{i}}{2}\omega(y, y')}\hat{W}(y + y'). \tag{7.37}$$

We say that it is *regular* if

$$t \mapsto \hat{W}(ty)$$

is strongly continuous for any $y \in \mathcal{Y}$.

One of the main examples of regular CCR representations is the Schrödinger representation

$$\mathbb{R}^n \oplus \mathbb{R}^n \ni (\xi, \eta) \mapsto \hat{W}(\xi, \eta) := \mathrm{e}^{\mathrm{i}(\hat{x}(\xi) + \hat{p}(\eta))} \in U\big(L^2(\mathbb{R}^n)\big). \tag{7.38}$$

In this case $\mathcal{Y} = \mathbb{R}^n \oplus \mathbb{R}^n$, $y = (\xi, \eta)$, $y' = (\xi', \eta')$,

$$\omega(y, y') = \xi\eta' - \eta\xi'. \tag{7.39}$$

If $\mathcal{Y}$ is a finite dimensional symplectic space, then its dimension is necessarily even and we can find a basis so that the symplectic form is (7.39). The Stone-von Neumann theorem says that every irreducible strongly continuous CCR representation over a finite dimensional symplectic space is unitarily equivalent to a multiple of the Schrödinger representation.

Note that if we have a regular CCR representation over $\mathcal{Y}$ and $y \in \mathcal{Y}$, then

$$\mathbb{R} \ni t \mapsto \hat{W}(ty) \in U(\mathcal{H}) \tag{7.40}$$

is a 1-parameter unitary group. Hence it has a generator, which will be denoted $\hat{\phi}(y)$, so that

$$\hat{W}(ty) = \mathrm{e}^{\mathrm{i}t\hat{\phi}(y)}. \tag{7.41}$$

It is easy to show that on an appropriate domain

$$\hat{\phi}(ty) = t\hat{\phi}(y), \tag{7.42}$$

$$\hat{\phi}(y + y') = \hat{\phi}(y) + \hat{\phi}(y'), \tag{7.43}$$

$$[\hat{\phi}(y), \hat{\phi}(y')] = \mathrm{i}\omega(y, y'). \tag{7.44}$$

We can also extend these "fields" to the complexification of $\mathcal{Y}$, denoted $\mathbb{C}\mathcal{Y} := \mathcal{Y} + \mathrm{i}\mathcal{Y}$, that is consisting of $y = y_{\mathrm{R}} + \mathrm{i}y_{\mathrm{I}}$, $y_{\mathrm{R}}, y_{\mathrm{I}} \in \mathcal{Y}$. Note that we have the complex conjugation $\overline{y} := y_{\mathrm{R}} - \mathrm{i}y_{\mathrm{I}}$. We set

$$\hat{\phi}(y) := \hat{\phi}(y_{\mathrm{R}}) + \mathrm{i}\hat{\phi}(y_{\mathrm{I}}). \tag{7.45}$$

Clearly, $\hat{\phi}(y)^* = \hat{\phi}(\overline{y})$.

There are many irregular CCR representations. For instance, we can consider $l^2(\mathcal{Y})$ with basis $\{e_y \mid y \in \mathcal{Y}\}$ and

$$\hat{W}(y)e_{y'} = \mathrm{e}^{-\frac{\mathrm{i}}{2}y\cdot\omega y'}e_{y+y'}. \tag{7.46}$$

Usually, they are only a non-physical mathematical curiosity.

7.7 Fock representations of the CCR

Let $\mathcal{Z}$ be a Hilbert space. It is then a symplectic space with the form

$$\omega(z, z') := 2\mathrm{Im}(z|z'). \tag{7.47}$$

Set

$$\hat{W}(z) := \mathrm{e}^{\hat{a}^*(z) - \hat{a}(z)}. \tag{7.48}$$

Then, using the Baker-Campbell-Hausdorff formula we see that

$$\mathcal{Z} \ni z \mapsto \hat{W}(z) \in U\big(\Gamma_{\mathrm{s}}(\mathcal{Z})\big) \tag{7.49}$$

is a regular irreducible CCR representation over the symplectic space $\mathcal{Z}$. Of course, if $\mathcal{Z}$ is finite dimensional, it is unitarily equivalent to the Schrödinger representation, which follows from the Stone-von Neumann Theorem, but is also an obvious consequence of the well known theory of the harmonic oscillator.

We have

$$\hat{W}(z) = \mathrm{e}^{-\frac{(z|z)}{2}} \mathrm{e}^{\hat{a}^*(z)} \mathrm{e}^{-\hat{a}(z)}, \tag{7.50}$$

$$\hat{a}(z)\Omega = 0, \quad z \in \mathcal{Z}. \tag{7.51}$$

Hence,

$$(\Omega|\hat{W}(z)\Omega) = \mathrm{e}^{-\frac{(z|z)}{2}}. \tag{7.52}$$

Therefore, if we know the vacuum state we can recover the real part of the scalar product on $\mathcal{Z}$.

The symplectic form ω fixes the imaginary part of the scalar product, see (7.47). Then there are many ways you can complete it to a full scalar product. Each of them leads to a Fock representation of CCR satisfying (7.52). If $\mathcal{Z}$ has an infinite dimension, the resulting representations in general will not be unitarily equivalent, as we will illustrate in the next section.

7.8 Equivalence of representations of CCR

Suppose that $(\mathcal{Y}, \omega)$ is a symplectic space and $\mathcal{Y} \ni y \mapsto W_i(y) \in U(\mathcal{H}_i)$, $i = 1, 2$ are two representations of CCR. We say that they are unitarily equivalent if there exists a unitary $U : \mathcal{H}_1 \to \mathcal{H}_2$ such that

$$UW_1(y) = W_2(y)U, \quad y \in \mathcal{Y}. \tag{7.53}$$

The Stone-von Neumann Theorem says that all CCR representations over a finite dimensional symplectic space are unitarily equivalent up to a multiplicity. This is not the case for an infinite number of degrees of freedom.

In fact, for instance, there are many inequivalent Fock representations over the same infinite dimensional symplectic space.

Let us do a computation that illustrates this. Let us start with the symplectic space $\mathbb{R}^2$ with the Schrödinger representation on $L^2(\mathbb{R})$ given by $\hat{x}$, $\hat{p}$. For any $\omega > 0$ we introduce the creation/annihilation operators

$$a^*_\omega := \frac{1}{\sqrt{2}}\Big(\sqrt{\omega}\hat{x} - \frac{\mathrm{i}\hat{p}}{\sqrt{\omega}}\Big), \quad a_\omega := \frac{1}{\sqrt{2}}\Big(\sqrt{\omega}\hat{x} + \frac{\mathrm{i}\hat{p}}{\sqrt{\omega}}\Big). \tag{7.54}$$

The vacuum annihilated by a_ω is

$$\Omega_\omega(x) = \frac{\sqrt[4]{\omega}}{\sqrt[4]{\pi}} \mathrm{e}^{-\frac{\omega x^2}{2}}. \tag{7.55}$$

The vectors

$$e_{\omega,n} := \frac{1}{\sqrt{n!}} a^{*n}_\omega \Omega_\omega \tag{7.56}$$

form an orthonormal basis of eigenvectors of the harmonic ascillator a^*a. Thus

$$U_\omega \Phi := \sum_{n=0}^{\infty} |n)(e_{\omega,n}|\Phi) \tag{7.57}$$

is a unitary operator $U_\omega : L^2(\mathbb{R}) \to \Gamma_{\rm s}(\mathbb{C}) \sim l^2(0,1,2,\dots)$. We have

$$\hat{x} = \frac{1}{\sqrt{2\omega}}(a_\omega^* + a_\omega), \quad \hat{p} = \mathrm{i}\frac{\sqrt{\omega}}{\sqrt{2}}(a_\omega^* - a_\omega). \tag{7.58}$$

Obviously, these representation are unitarily equivalent. In fact, setting

$$V_\omega \Phi(x) := \sqrt[4]{\omega}\Phi(\sqrt{\omega}x), \tag{7.59}$$

we obtain

$$V_\omega \hat{x} V_\omega^{-1} = \sqrt{\omega}\hat{x}, \quad V_\omega \hat{p} V_\omega^{-1} = \frac{1}{\sqrt{\omega}}\hat{p}, \tag{7.60}$$

hence

$$V_\omega \hat{a}_1^* V_\omega^{-1} = \hat{a}_\omega^*, \quad V_\omega \hat{a}_1 V_\omega^{-1} = \hat{a}_\omega, \quad V_\omega e_{1,n} = e_{\omega,n}, \tag{7.61}$$

and $V_\omega = U_\omega^{-1} U_1$. We can also compute

$$(\Omega_\omega|\Omega_1) = \sqrt{\frac{2}{\omega^{\frac{1}{2}} + \omega^{-\frac{1}{2}}}}. \tag{7.62}$$

So far we treated $L^2(\mathbb{R})$ as the underlying space. Let us now treat the Fock space $\Gamma_{\rm s}(\mathbb{C})$ as the main space. Then for any $\omega > 0$ we have a Fock representation

$$\mathbb{R}^2 \ni (\xi,\eta) \mapsto W_\omega(\xi,\eta) := \exp\Big(\frac{\mathrm{i}\xi}{\sqrt{2\omega}}(a^* + a) + \frac{\mathrm{i}\eta\sqrt{\omega}}{\sqrt{2}}(a^* - a)\Big). \tag{7.63}$$

They are different, but unitarily equivalent.

It is straightforward to generalize this construction to a finite number of degrees of freedom. Thus, for any finite sequence of positive numbers we obtain the equivalence of two CCR representations of the symplectic space $\mathbb{R}^{2n}$: the Schrödinger representation on $L^2(\mathbb{R}^n)$ and the Fock representation on $\Gamma_{\rm s}(\mathbb{C}^n)$. The vacua corresponding to $\omega = (\omega_1,\dots,\omega_n)$ and $1 = (1,\dots,1)$ have a positive scalar product:

$$(\Omega_\omega|\Omega_1) = \prod_{j=1}^{n} \sqrt{\frac{2}{\omega_j^{\frac{1}{2}} + \omega_j^{-\frac{1}{2}}}} > 0. \tag{7.64}$$

The Schrödinger representation does not work for $n = \infty$, since there is no generalization of the Lebesgue measure to $\mathbb{R}^\infty$. However, the Fock space $\Gamma_{\rm s}(l^2)$ is well defined. Thus we can define creation/annihilation operators a_i^*, a_j, $i = 1,2,\dots$.

For any infinite sequence $\omega = (\omega_1, \omega_2, \dots)$ we can represent the commutation relations

$$[\hat{x}_i, \hat{p}_j] = \mathrm{i}\delta_{ij} \tag{7.65}$$

by setting

$$\hat{x}_{\omega,i} = \frac{1}{\sqrt{2\omega_i}}(a_i^* + a_i), \quad \hat{p}_{\omega,i} = \mathrm{i}\frac{\sqrt{\omega_i}}{\sqrt{2}}(a_i^* - a_i). \tag{7.66}$$

However, if $1 = (1, 1 \dots, \dots)$, the infinite product

$$(\Omega_\omega | \Omega_1) = \prod_{j=1}^{\infty} \sqrt{\frac{2}{\omega_j^{\frac{1}{2}} + \omega_j^{-\frac{1}{2}}}}. \tag{7.67}$$

is usually zero. One can show that if (7.67) is zero then the representations given by ω and 1 are inequivalent.

7.9 Two steps of quantization with an infinite number of degrees of freedom

Description of quantum systems with an infinite number of degrees of freedom (especially free systems) usually proceeds in two steps.

1. First one describes the symplectic space of classical fields. This automatically fixes commutation relations satisfied by quantum fields.

2. Then one chooses a Hilbert space where the quantum fields are represented. (Typically, this is a Fock space)

In the mathematically oriented literature there exist several equvalent ways of presenting CCR relations. Probably, the most economical way involves the notion of a CCR representation, which we introduced above. An alternative way is to use a $*$ algebra of CCR. Then the two steps described above can be described as foillows:

1. Introduce an abstract $*$-algebra of CCR over the space $(\mathcal{Y}, \omega)$.

2. Find a representation of this algebra.

This approach has a minor problem: there are several, essentially equivalent but mathematically different $*$-algebras that can be used to describe Canonical Commutation Relations. Let us describe two of them (there are others).

The *"Weyl CCR C^*-algebra"* is the C^* algebra generated by $\{\hat{W}(y) \mid y \in \mathcal{Y}\}$ satisfying

$$\hat{W}(y)^* = \hat{W}(-y), \quad \hat{W}(0) = \mathbb{1}, \tag{7.68}$$

$$\hat{W}(y)\hat{W}(y') = \mathrm{e}^{-\frac{\mathrm{i}}{2}y\cdot\omega y'}\hat{W}(y + y'). \tag{7.69}$$

The *"field CCR $*$-algebra"* is the $*$-algebra generated by $\{\hat{\phi}(y) \mid y \in \mathcal{Y}\}$ satisfying

$$\hat{\phi}(\alpha y + \alpha' y') = \alpha\hat{\phi}(y) + \alpha'\hat{\phi}(y'), \quad \hat{\phi}(y)^* = \hat{\phi}(y), \tag{7.70}$$

$$[\hat{\phi}(y), \hat{\phi}(y')] = \mathrm{i}y \cdot \omega y' \mathbb{1}. \tag{7.71}$$

The advantage of the Weyl CCR C^*-algebra is that it is a true C^*-algebra, hence it is prefered by numerous "C^*-algebras lovers". It also allows us to consider irregular representations. On the other hand, it consists of "almost periodic functions on the phase space", whose physical significance can be doubted.

The *"field CCR $*$-algebra"* seems "closer to the physics". However, it is not a C^*-algebra, and its representations involve unbounded operators, which could be problematic.

The second step of quantization, that is fixing a representation, can be performed by fixing a state, and then using the GNS representation. For instance, the Fock state σ in the setting of Subsection 7.7 is given by

$$\sigma(\hat{W}(z)) = \mathrm{e}^{-\frac{(z|z)}{2}}. \tag{7.72}$$

The GNS representation wrt σ acts naturally in the bosonic Fock space, as described in Subsection 7.7. The state σ corresponds to the Fock vacuum: $\sigma = (\Omega| \cdot \Omega)$.

7.10 Positive energy Fock quantization

Consider a quadratic Hamiltonian on a phase space $\mathcal{Y}$. If we fix coordinate functions ϕ^i, it can be written as

$$H = \frac{1}{2}\sum_{i,j} h_{ij}\phi^i\phi^j \tag{7.73}$$

for some symmetric matrix $[h_{ij}]$. As we discussed above, if $\mathcal{Y}$ is finite dimensional, we could quantize H as

$$\hat{H}^{\mathrm{sym}} = \frac{1}{2}\sum_{i,j} h_{ij}\hat{\phi}^i\hat{\phi}^j. \tag{7.74}$$

Because of a finite number of degrees of freedom this is well defined and essentially unique, since all irreducible representations are equivalent, so that this quantization is essentially unique.

If the number of degrees of freedom is infinite, usually only the phase space with its symplectic structure is given beforehand. In the quantum theory one also needs a CCR representation on a Hilbert space, which is less canonical and more tricky to choose. How to select a physically motivated CCR representation, if we are given a symplectic space?

Suppose that the symplectic form is given by the matrix $[\omega_{ij}]$, with its inverse denoted $[\omega^{ij}]$. This is expressed by two equivalent identities, one for the symplectic form, the other for the Poisson bracket:

$$\omega = \sum_{ij} \omega_{ij} \phi^i \otimes \phi^j = \frac{1}{2} \omega_{ij} \phi^i \wedge \phi^j; \tag{7.75}$$

$$\{\phi^i, \phi^j\} = \omega^{ij}. \tag{7.76}$$

Introduce the operator $k := \omega^{-1} h$, or

$$k^i_j := \omega^{ik} h_{kj}. \tag{7.77}$$

For $\zeta \in \mathbb{R}^{2n}$, note that $k\zeta = \omega^{-1} \mathrm{d}H(\zeta)$ is the Hamiltonian vector field generated by H. Thus the dynamics generated by H is $r_t = \mathrm{e}^{tk}$. Thus on the classical level we have the dynamics $t \mapsto \phi^i(t)$ with $\phi^i(0) = \phi^i$ is given by the linear transformation

$$\phi^i(t) = r^i_{t,j} \phi_j. \tag{7.78}$$

We would like to have a quantization, such that the analogous identity is true on the quantum level. In other words, we would like to have a Hilbert space $\mathcal{H}$ equipped with operators $\hat{\phi}^i$ and $\hat{H}$ such that

$$\mathrm{e}^{\mathrm{i}t\hat{H}} \hat{\phi}^i \mathrm{e}^{-\mathrm{i}t\hat{H}} = r^i_{t,j} \hat{\phi}_j. \tag{7.79}$$

If the number of degrees of freedom is finite this is achieved by (7.74). We can also subtract from (7.74) any real number and (7.79) will still hold.

Let us now assume that H is strictly positive. We will describe the whole procedure as if the number of degrees of freedom were finite, so that $\mathcal{Y} = \mathbb{R}^{2n}$, but it is easy to generalize it to the general case.

The matrix $[h_{ij}]$ defining the Hamiltonian can be used to fix a sesquilinear scalar product on the complexification of the phase space, that is on $\mathbb{C}^{2n}$:

$$\overline{\zeta}^i h_{ij} \xi^j =: \langle \overline{\zeta} | h \xi \rangle, \tag{7.80}$$

Note that $-\mathrm{i}k$ is self-adjoint in the scalar product (7.80). Therefore, we can diagonalize $-\mathrm{i}k$ in a basis orthonormal in (7.80). Note that all eigenvalues of $-\mathrm{i}k$ are nonzero and real. Besides, if $\overline{v}_i$ is an eigenvector of $-\mathrm{i}k$ with eigenvalue ε_i, then v_i is an eigenvector with eigenvalue $-\varepsilon_i$, because $-\mathrm{i}k$ is purely imaginary. Thus

$$\langle \overline{\zeta} | h \xi \rangle = \sum_i \big(\langle \overline{\zeta} | h \overline{v}_i \rangle \langle v_i | h \xi \rangle + \langle \overline{\zeta} | h v_i \rangle \langle \overline{v}_i | h \xi \rangle \big), \tag{7.81}$$

$$\mathrm{i} \langle \overline{\zeta} | \omega \xi \rangle = \langle \overline{\zeta} | h (-\mathrm{i}k)^{-1} \xi \rangle = \sum_i \varepsilon_i^{-1} \big(\langle \overline{\zeta}_i | h \overline{v}_i \rangle \langle v_i | h \xi \rangle - \langle \overline{\zeta}_i | h v_i \rangle \langle \overline{v}_i | h \xi \rangle \big),$$

where we can assume that all ε_i are positive. Introduce the following functionals acting on real vectors ζ:

$$\langle a_i|\zeta\rangle := \frac{1}{\sqrt{\varepsilon_i}}\langle v_i|h\zeta\rangle, \tag{7.82}$$

$$\langle a_i^*|\zeta\rangle := \frac{1}{\sqrt{\varepsilon_i}}\langle \overline{v}_i|h\zeta\rangle = \frac{1}{\sqrt{\varepsilon_i}}\overline{\langle v_i|h\zeta\rangle}. \tag{7.83}$$

Then for real ζ, ξ (7.81) yields

$$\langle H|\zeta\rangle = \sum_i \varepsilon_i \langle a_i^*|\zeta\rangle\langle a_i|\zeta\rangle, \tag{7.84}$$

$$\mathrm{i}\langle\overline{\zeta}|\omega\xi\rangle = \langle\overline{\zeta}|h(-\mathrm{i}k)^{-1}\xi\rangle = \sum_i \big(\langle a_i^*|\zeta\rangle\langle a_i|\xi\rangle - \langle a_i|\zeta\rangle\langle a_i^*|\xi\rangle\big),$$

which can be rewritten as

$$H = \sum \varepsilon_i a_i^* a_i, \tag{7.85}$$

$$\mathrm{i}\omega = \sum a_i^* \wedge a_i, \tag{7.86}$$

where the last line is equivalent to

$$\{a_i, a_j^*\} = -\mathrm{i}\delta_{ij}, \qquad \{a_i, a_j\} = \{a_i^*, a_j^*\} = 0. \tag{7.87}$$

Now we quantize the fields on a Hilbert space with the vector Ω, so that

$$[\hat{a}_i, \hat{a}_j^*\} = \delta_{ij}, \qquad [\hat{a}_i, \hat{a}_j] = [\hat{a}_i^*, \hat{a}_j^*] = 0, \quad \hat{a}_i\Omega = 0. \tag{7.88}$$

Clearly, what we obtain is the bosonic space with the 1-particle space spanned by $\hat{a}_i^*\Omega$. We choose the Hamiltonian

$$\hat{H} = \sum \varepsilon_i \hat{a}_i^* \hat{a}_i. \tag{7.89}$$

Note that $\hat{H}$ is positive, $\hat{H}\Omega = 0$ and (7.79) holds. If $\hat{H}^{\mathrm{sym}}$ is well defined, then it differs from $\hat{H}$ by a constant $\frac{1}{2}\sum\lambda_i$.

Let us now describe the above procedure in a basis independent way. Suppose that H is a positive quadratic form on a real vector space $\mathcal{Y}$ equipped with a symplectic form ω. We first extend H to a bilinear form on $\mathcal{Y}$ by polarization identity. This form is generated by an operator from $\mathcal{Y}$ to the dual of $\mathcal{Y}$, which we denote by h

$$\langle\zeta|h\xi\rangle := H(\zeta+\xi) - H(\zeta) - H(\xi), \quad \zeta, \xi \in \mathcal{Y}. \tag{7.90}$$

Equivalently, $h\zeta = \mathrm{d}H(\zeta)$. Thus $H(\zeta) = \frac{1}{2}\langle\zeta|h\zeta\rangle$ and for $k := \omega^{-1}h$, the symplectic dynamics is $r_t = \mathrm{e}^{tk}$.

We extend h and $\mathrm{i}\omega$ as maps from $\mathbb{C}\mathcal{Y}$ to the dual of $\mathbb{C}\mathcal{Y}$. We consider the sesquilinear forms

$$\langle\overline{\zeta}|h\zeta\rangle \tag{7.91}$$

as a scalar product on $\mathbb{C}\mathcal{Y}$ called the *energy scalar product*. We easily check that $-\mathrm{i}k$ is a self-adjoint operator on $\mathbb{C}\mathcal{Y}$. We can diagonalize $-\mathrm{i}k$. Because of nondegeneracy of ω, this operator has a zero nullspace. Hence we have also a nondegenerate sesquilinear form

$$\mathrm{i}\langle\overline{\zeta}|\omega\zeta\rangle = \langle\overline{\zeta}|h(-\mathrm{i}k)^{-1}\zeta\rangle$$

Let $\mathcal{W}^{(+)}$ and $\mathcal{W}^{(-)}$ be the positive and negative subspace of $\mathbb{C}\mathcal{Y}$ of the self-adjoint operator $-\mathrm{i}k$. We have

$$\overline{\mathcal{W}^{(+)}} = \mathcal{W}^{(-)}, \tag{7.92}$$

$\mathrm{i}\omega$ endows $\mathcal{Z} := \mathcal{W}^{(+)}$ with the positive scalar product

$$(z|z') = \mathrm{i}\langle\overline{z}|\omega z'\rangle \tag{7.93}$$

and $-\mathrm{i}k$ is self-adjoint wrt (7.93). Let us set

$$\hat{H} := \mathrm{d}\Gamma\Big(-\mathrm{i}k\big|_{\mathcal{Z}}\Big). \tag{7.94}$$

We have

$$\mathrm{e}^{\mathrm{i}t\hat{H}}W(z)\mathrm{e}^{-\mathrm{i}t\hat{H}} = W(\mathrm{e}^{tk}z), \quad z \in \mathcal{Z}. \tag{7.95}$$

The scalar product (7.93) will be treated as the basic one on $\mathcal{Z}$ and called the *dynamical scalar product*. We have

$$\langle\overline{z}|hz'\rangle = (z|-\mathrm{i}kz'). \tag{7.96}$$

Thus using $(\cdot|\cdot)$ we can identify $-\mathrm{i}k$ restricted to $\mathcal{Z}$ with h restricted to $\mathcal{Z}$.

The above construction guarantees that

(1) There exists a unitary group on the Hilbert space $\Gamma_{\mathrm{s}}(\mathcal{Z})$ that implements the dynamics, see (7.95).

(2) The Hamiltonian $\hat{H}$ generating the dynamics is positive, because $h\Big|_{\mathcal{Z}}$ is positive.

(3) The Fock vacuum Ω is a nondegenerate ground state of the Hamitonian.

7.11 Positive energy quantization for charged systems

Suppose that the symplectic space $\mathcal{Y}$ is equipped with a $U(1)$ symmetry. More precisely, we assume that it is $\mathcal{Y} = \mathcal{Y}_{\mathrm{R}} \oplus \mathcal{Y}_{\mathrm{I}}$ and its coordinates are spanned by ϕ^i_{R}, ϕ^i_{I} satisfying

$$\{\phi^i_{\mathrm{R}}, \phi^j_{\mathrm{R}}\} = \omega^{ij}, \quad \{\phi^i_{\mathrm{I}}, \phi^j_{\mathrm{I}}\} = \omega^{ij}, \quad \{\phi^i_{\mathrm{R}}, \phi^j_{\mathrm{I}}\} = 0, \tag{7.97}$$

for some symplectic matrix ω on $\mathcal{Y}_{\mathrm{R}} \simeq \mathcal{Y}_{\mathrm{I}}$. The element $\mathrm{e}^{\mathrm{i}\theta} \in U(1)$ acts on the coordinates as

$$\phi^i_{\mathrm{R}} \mapsto \cos\theta\phi^i_{\mathrm{R}} - \sin\theta\phi^i_{\mathrm{I}}, \quad \phi^i_{\mathrm{R}} \mapsto \sin\theta\phi^i_{\mathrm{R}} + \cos\theta\phi^i_{\mathrm{I}}. \tag{7.98}$$

In such a case it is customary to treat the space $\mathcal{Y}$ as a complex space $\mathcal{Y} = \mathbb{C}\mathcal{Y}_{\mathrm{R}}$, setting

$$\psi^i = \frac{1}{\sqrt{2}}(\phi^i_{\mathrm{R}} + \mathrm{i}\phi^i_{\mathrm{I}}), \quad \psi^{i*} = \frac{1}{\sqrt{2}}(\phi^i_{\mathrm{R}} - \mathrm{i}\phi^i_{\mathrm{I}}), \tag{7.99}$$

so that

$$\{\psi^i, \psi^j\} = \{\psi^{i*}, \psi^{j*}\} = 0, \quad \{\psi^i, \psi^{j*}\} = -\omega^{ij}, \tag{7.100}$$

and the action of the group is $\psi^i \mapsto \mathrm{e}^{\mathrm{i}\theta}\psi^i$, $\psi^{i*} \mapsto \mathrm{e}^{-\mathrm{i}\theta}\psi^{i*}$.

Note that the space $\mathcal{Y}$ is equipped with complex conjugation c. It satisfies $c\psi^i c = \psi^{i*}$, $c^2 = \mathbb{1}$. It can be interpreted as the charge conjugation.

Suppose that H is a (real) quadratic Hamiltonian that is invariant wrt $U(1)$. Then it can be written as

$$H = \sum_{ij} h_{ij}\psi^{i*}\psi^j \tag{7.101}$$

for some Hermitian matrix $[h_{ij}]$. The symplectic form leads to the following sesquilinear form, which will be called the *charge*:

$$Q = \mathrm{i}\sum_{ij} \omega_{ij}\psi^{i*}\psi^j \tag{7.102}$$

We diagonalize simultaneously H and Q obtaining $I = I_+ \sqcup I_-$

$$H = \sum_{i\in I} \varepsilon_i a_i^* a_i, \tag{7.103}$$

$$Q = \sum_{i\in I_+} a_i^* a_i - \sum_{i\in I_-} a_i^* a_i, \tag{7.104}$$

$$\{a_i, a_j^*\} = 0, \quad i \neq j, \qquad \{a_i, a_i^*\} = \mp\mathrm{i}, \quad i \in I_\pm. \tag{7.105}$$

(Note that (7.104) and (7.105) are equivalent). We rename $a_i = b_i^*$, $a_i^* = b_i$ for $i \in I_-$. Thus

$$H = \sum_{i\in I_+} \varepsilon_i a_i^* a_i + \sum_{i\in I_-} \varepsilon_i b_i^* b_i, \tag{7.106}$$

$$Q = \sum_{i\in I_+} a_i^* a_i - \sum_{i\in I_-} b_i^* b_i, \tag{7.107}$$

$$\{a_i, a_j^*\} = \{b_i, b_j^*\} = -\mathrm{i}\delta_{ij}. \tag{7.108}$$

Note that the space $\mathcal{Y} = \mathcal{Y}_+ \oplus \mathcal{Y}_-$.

The quantization of this system yields $\Gamma_{\mathrm{s}}(\mathcal{Y}_+ \oplus c\mathcal{Y}_-)$. The Hamiltonian and charge are

$$\hat{H} = \mathrm{d}\Gamma\Big(h\Big|_{\mathcal{Y}_+} \oplus chc\Big|_{c\mathcal{Y}_-}\Big), \quad \hat{Q} = \mathrm{d}\Gamma\Big(\mathbb{1}\Big|_{\mathcal{Y}_+} \oplus -\mathbb{1}\Big|_{c\mathcal{Y}_-}\Big).$$

The quantized charge conjugation is $\hat{C} := \mathrm{d}\Gamma(c)$

If in addition the matrix $[h_{ij}]$ is real then we have

$$H = \frac{1}{2}\sum_{ij} h_{ij}\left(\phi^i_{\mathrm{R}}\phi^j_{\mathrm{R}} + \phi^i_{\mathrm{I}}\phi^j_{\mathrm{I}}\right) \tag{7.109}$$

Clearly, then $H = H \circ c$, $Q = -Q \circ c$ Then then we can choose the diagonalizing functionals so that $ca_i c = b_i$, $ca_i^* c = b_i^*$.

After quantization we have $\hat{C}\hat{a}_i\hat{C} = \hat{b}_i$, $\hat{C}\hat{a}_i^*\hat{C} = \hat{b}_i^*$, $\hat{C}\hat{H}\hat{C} = \hat{H}$, $\hat{C}\hat{Q}\hat{C} = -\hat{Q}$.

8 Free neutral scalar bosons

8.1 Classical fields off-shell and on-shell

Consider the Minkowski space $\mathbb{R}^{13}$. In the off-shell formalism a field configuration is a function $\mathbb{R}^{1,3} \ni x \mapsto \zeta(x)$. A field configuration ζ satisfies the Klein-Gordon equation if

$$(-\Box + m^2)\zeta(x) = 0. \tag{8.1}$$

The field in the off-shell formalism is the functional on, say, real smooth functions on $\mathbb{R}^{1,3}$, such that

$$\langle\phi(x)|f\rangle := f(x), \quad f \in C^\infty(\mathbb{R}^{1,3}, \mathbb{R}). \tag{8.2}$$

(The choice of smooth functions does not matter much, since the Lagrangian formalism serves mainly to obtain formal identities). Recall that to obtain a field equation one chooses a local *Lagrangian density* $\mathcal{L}(x)$, which is a function of the field $\phi(x)$, $\partial_\mu\phi(x) =: \phi_{,\mu}(x)$ and of $x \in \mathbb{R}^{1,3}$. The *Euler-Lagrange equation* reads then

$$\partial_{\phi(x)}\mathcal{L}(x) - \partial_\mu \frac{\partial\mathcal{L}(x)}{\partial\phi_{,\mu}(x)} = 0 \tag{8.3}$$

To obtain the Klein-Gordon equation (8.1), we use the Lagrangian density

$$\mathcal{L}(x) = \quad -\tfrac{1}{2}\partial_\mu\phi(x)\partial^\mu\phi(x) - \tfrac{1}{2}m^2\phi(x)^2. \tag{8.4}$$

The Euler-Lagrange equation then yields

$$(-\Box + m^2)\phi(x) = 0. \tag{8.5}$$

Let $\zeta \in C^\infty(\mathbb{R}^{1,3})$ solve the Klein-Gordon equation (8.1) and let $\mathrm{supp}\zeta \cap \mathbb{R}^3$ be compact. Recall the identity (4.33):

$$\zeta(t,\vec{x}) = \quad \int_{\mathbb{R}^3} \dot{G}^{\mathrm{PJ}}(t,\vec{x}-\vec{y})\zeta(0,\vec{y})\mathrm{d}\vec{y} + \int_{\mathbb{R}^3} G^{\mathrm{PJ}}(t,\vec{x}-\vec{y})\dot{\zeta}(0,\vec{y})\mathrm{d}\vec{y}. \tag{8.6}$$

Recall that a function on $\mathbb{R}^{1,3}$ is called *space compact* if there exists a compact $K \subset \mathbb{R}^{1,n}$ such that $\mathrm{supp}f \subset J(K)$. The set of space compact smooth

functions will be denoted $C^\infty_{\rm sc}(\mathbb{R}^{1,3})$. Therefore all solutions of (8.1) with compactly supported Cauchy data are space compact.

Let $\mathcal{Y}_{\rm KG}$ denote the *space of real*, resp. *space-compact solutions of the Klein-Gordon equation* We can endow the space $\mathcal{Y}_{\rm KG}$ with the standard topology of $C^\infty_{\rm c}(\mathbb{R}^3)\oplus C^\infty_{\rm c}(\mathbb{R}^3)$ given by the initial conditions. The space of real continuous functionals on $\mathcal{Y}_{\rm KG}$ will be denoted by $\mathcal{Y}^{\rm T}_{\rm KG}$. The action of $T\in\mathbb{C}\mathcal{Y}^{\rm T}_{\rm KG}$ on $\zeta\in\mathcal{Y}_{\rm KG}$ will be denoted by $\langle T|\zeta\rangle$, and sometimes simply by $T\zeta$.

The field $\phi(x)$ understood as (8.2) will be called an *off-shell field*. It is used in the Lagrangian formalism. When we go from the Lagrangian to Hamiltonian formalism, we enforce the *on-shell* condition, that is, we restrict ourselves to solutions of the E-L equation. We are usually also more careful in the choice of the space on which the fields act: we restrict ourselves to $\mathcal{Y}_{\rm KG}$. Thus, for $x\in\mathbb{R}^{1,3}$, the on-shell field $\phi(x)$ acting on $\zeta\in\mathcal{Y}_{\rm KG}$ gives

$$\langle\phi(x)|\zeta\rangle := \zeta(x),$$

We will not distinguish the notation for on-shell and off-shell fields.

Clearly, for any $\zeta\in\mathcal{Y}_{\rm KG}$ we have

$$(-\Box+m^2)\langle\phi(x)|\zeta\rangle = 0.$$

Thus the equation (8.5) for on-shell fields is a tautology.

In the on-shell formalism we also introduce the variable conjugate to $\phi(x)$:

$$\pi(x) \;:=\; \frac{\partial\mathcal{L}(x)}{\partial\phi_{,0}(x)} = \phi_{,0}(x) = \dot\phi(x). \tag{8.7}$$

By (8.6),

$$\phi(t,\vec x) = \int \dot G^{\rm PJ}(t,\vec x-\vec y)\phi(0,\vec y)\mathrm{d}\vec y + \int G^{\rm PJ}(t,\vec x-\vec y)\pi(0,\vec y)\mathrm{d}\vec y. \tag{8.8}$$

The Poincaré group $\mathbb{R}^{1,3}\rtimes O(1,3)$ acts on $\mathcal{Y}_{\rm KG}$ by

$$r_{(y,\Lambda)}\zeta(x) := \zeta\left((y,\Lambda)^{-1}x\right).$$

Equivalently,

$$r^{\rm T-1}_{(y,\Lambda)}\phi(x) = \phi(\Lambda x+y). \tag{8.9}$$

8.2 Symplectic form and Poisson bracket

For $\zeta_1,\zeta_2\in C^\infty_{\rm sc}(\mathbb{R}^{1,3})$ we define

$$j^\mu(x,\zeta_1,\zeta_2) \;:=\; \partial^\mu\zeta_1(x)\zeta_2(x) - \zeta_1(x)\partial^\mu\zeta_2(x). \tag{8.10}$$

Writing $j^\mu(x)$ for brevity, we easily check that

$$\partial_\mu j^\mu(x) = (\Box-m^2)\zeta_1(x)\zeta_2(x) - \zeta_1(x)(\Box-m^2)\zeta_2(x),$$

This implies Green's identity

$$\int j^0(t_+,\vec{x})\mathrm{d}\vec{x} - \int j^0(t_-,\vec{x})\mathrm{d}\vec{x} \tag{8.11}$$

$$= \int_{t_-<x^0<t_+} \Big((-\Box+m^2)\zeta_1(x)\zeta_2(x) - \zeta_1(x)(-\Box+m^2)\zeta_2(x)\Big)\mathrm{d}x. \tag{8.12}$$

Thus if $\zeta_1,\zeta_2\in\mathcal{Y}_{\mathrm{KG}}$, then

$$\partial_\mu j^\mu(x) = 0.$$

One says that $j^\mu(x)$ is a *conserved 4-current*.

A space-like subspace of codimension 1 will be called a *Cauchy subspace*. The flux of j^μ across any Cauchy subspace $\mathcal{S}$ does not depend on its choice. It defines a *symplectic form* on $\mathcal{Y}_{\mathrm{KG}}$

$$\begin{aligned}\omega(\zeta_1,\zeta_2) &= \int_{\mathcal{S}} j^\mu(x,\zeta_1,\zeta_2)\mathrm{d}s_\mu(x)\\ &= \int \Big(-\dot{\zeta}_1(t,\vec{x})\zeta_2(t,\vec{x}) + \zeta_1(t,\vec{x})\dot{\zeta}_2(t,\vec{x})\Big)\,\mathrm{d}\vec{x}.\end{aligned} \tag{8.13}$$

Thus $(\mathcal{Y}_{\mathrm{KG}},\omega)$ is an (infinite dimensional) symplectic space.

Clearly, the form (8.13) is well defined also if only $\zeta_2\in\mathcal{Y}_{\mathrm{KG}}$, and ζ_1 is a distributional solution of the Klein-Gordon equation.

$r_{(y,\Lambda)}$ are symplectic (preserve the symplectic form) for $\Lambda\in O^\uparrow(1,3)$, otherwise they are antisymplectic (change the sign in front of the symplectic form).

By (8.13), the symplectic form can be written as

$$\omega(\zeta_1,\zeta_2) = \int \big(-\langle\pi(t,\vec{x})|\zeta_1\rangle\langle\phi(t,\vec{x})|\zeta_2\rangle + \langle\phi(t,\vec{x})|\zeta_1\rangle\langle\pi(t,\vec{x})|\zeta_2\rangle\big)\mathrm{d}\vec{x},$$

or more simply,

$$\omega = \int \phi(t,\vec{x})\wedge\pi(t,\vec{x})\mathrm{d}\vec{x}. \tag{8.14}$$

The conserved 4-current can be written as

$$j_\mu(x) = \phi(x)\wedge\partial_\mu\phi(x).$$

By (8.14), the symplectic structure on the space $\mathcal{Y}_{\mathrm{KG}}$ leads to the *Poisson bracket*

$$\begin{aligned}\{\phi(t,\vec{x}),\phi(t,\vec{y})\} = \{\pi(t,\vec{x}),\pi(t,\vec{y})\} &= 0,\\ \{\phi(t,\vec{x}),\pi(t,\vec{y})\} &= \delta(\vec{x}-\vec{y}).\end{aligned} \tag{8.15}$$

Using (8.8) we obtain

$$\{\phi(x),\phi(y)\} = -G^{\mathrm{PJ}}(x-y). \tag{8.16}$$

Therefore, the Pauli-Jordan solution is often called the *commutator function*.

The relations (8.15) can be viewed as mnemotechnic identities that yield the correct Poisson bracket for more regular functions, eg. the smeared out fields

$$\phi[f] := \int f(x)\phi(x)\mathrm{d}x. \tag{8.17}$$

We have

$$\{\phi[f], \phi[g]\} = -\int\int f(x)g(x)G^{\mathrm{PJ}}(x-y)\mathrm{d}x\mathrm{d}y. \tag{8.18}$$

Note that formally, for any $t \in \mathbb{R}$, $\phi(t,\vec{x})$ and $\pi(t,\vec{x})$ generate the algebra of all functions on $\mathcal{Y}_{\mathrm{KG}}$.

8.3 Stress-energy tensor

The Noether Theorem suggests to introduce the *stress-energy tensor*

$$\begin{aligned} \mathcal{T}^{\mu\nu}(x) &:= -\frac{\partial\mathcal{L}(x)}{\partial\phi_{,\mu}(x)}\phi^{,\nu}(x) + g^{\mu\nu}\mathcal{L}(x) \\ &= \partial^\mu\phi(x)\partial^\nu\phi(x) - g^{\mu\nu}\frac{1}{2}\left(\partial_\alpha\phi(x)\partial^\alpha\phi(x) + m^2\phi(x)^2\right). \end{aligned} \tag{8.19}$$

It is easy to check that the stress-energy tensor is conserved on solutions of the Klein-Gordon equation (on shell):

$$\partial_\mu\mathcal{T}^{\mu\nu}(x) = 0.$$

We express the stress-energy tensor in terms of $\phi(x)$ and $\pi(x)$. Its components with the first temporal coordinate are called the *Hamiltonian density* and *momentum density*:

$$\begin{aligned} \mathcal{H}(x) &:= \mathcal{T}^{00}(x) &&= \frac{1}{2}\left(\pi(x)^2 + \left(\vec{\partial}\phi(x)\right)^2 + m^2\phi(x)^2\right), \\ \mathcal{P}^i(x) &:= \mathcal{T}^{0i}(x) &&= -\pi(x)\partial^i\phi(x). \end{aligned}$$

They are examples of quadratic functionals on $\mathcal{Y}_{\mathrm{KG}}$: One easily checks

$$\{\phi(t,\vec{x}), \mathcal{H}(t,\vec{y})\} = \dot{\phi}(t,\vec{x})\delta(\vec{x}-\vec{y}), \tag{8.20}$$

$$\{\pi(t,\vec{x}), \mathcal{H}(t,\vec{y})\} = \dot{\pi}(t,\vec{x})\delta(\vec{x}-\vec{y}), \tag{8.21}$$

$$\{\phi(t,\vec{x}), \mathcal{P}^i(t,\vec{y})\} = -\partial^i\phi(t,\vec{x})\delta(\vec{x}-\vec{y}), \tag{8.22}$$

$$\{\pi(t,\vec{x}), \mathcal{P}^i(t,\vec{y})\} = -\partial^i\pi(t,\vec{x})\delta(\vec{x}-\vec{y}). \tag{8.23}$$

We introduce the *(total) Hamiltonian* and *momentum*:

$$H := \int_{\mathcal{S}} \mathcal{T}^{\mu 0}(x)\mathrm{d}s_\mu(x) = \int \mathcal{H}(t,\vec{x})\mathrm{d}\vec{x}, \tag{8.24}$$

$$P^i := \int_{\mathcal{S}} \mathcal{T}^{\mu i}(x)\mathrm{d}s_\mu(x) = \int \mathcal{P}^i(t,\vec{x})\mathrm{d}\vec{x}. \tag{8.25}$$

where $\mathcal{S}$ is any Cauchy subspace. They are examples of quadratic functionals:

$$\begin{aligned}\langle H|\zeta\rangle &= \int \frac{1}{2}\left(\dot{\zeta}(t,\vec{x})^2 + \left(\vec{\partial}\zeta(t,\vec{x})\right)^2 + m^2\zeta(t,\vec{x})^2\right),\\ \langle \mathcal{P}^i|\zeta\rangle &= -\int \dot{\zeta}(t,\vec{x})\partial^i\zeta(t,\vec{x}).\end{aligned}$$

H and $\vec{P}$ are the generators of the time and space translations:

$$\begin{aligned}\dot{\phi}(x) = \{\phi(x), H\}, \quad \dot{\pi}(x) = \{\pi(x), H\},\\ \vec{\partial}\phi(x) = -\{\phi(x), \vec{P}\}, \quad \vec{\partial}\pi(x) = -\{\pi(x), \vec{P}\}.\end{aligned}$$

The observables H, P^1, P^2 and P^3 are in involution. (This means that the Poisson bracket of every pair among these observables vanishes).

8.4 Simultaneous diagonalization of the symplectic form, Hamiltonian and momentum

If $T \in \mathcal{Y}_{\mathrm{KG}}^{\mathrm{T}}$, we define $T^* \in \mathcal{Y}_{\mathrm{KG}}^{\mathrm{T}}$ by

$$\langle T^*|\zeta\rangle := \overline{\langle T|\zeta\rangle}, \quad \zeta \in \mathcal{Y}_{\mathrm{KG}}.$$

Note that in this context the star does not denote the Hermitian conjugation (which in our text is the standard meaning of the star).

We can represent the field in terms of the Fourier transformation:

$$\phi(x) = (2\pi)^{-4}\int \mathrm{e}^{\mathrm{i}xk}\tilde{\phi}(k)\mathrm{d}k, \tag{8.26}$$

where because of the reality of $\mathcal{Y}_{\mathrm{KG}}$, $\tilde{\phi}(k)^* = \tilde{\phi}(-k)$. The Klein-Gordon equation implies

$$(k^2 + m^2)\tilde{\phi}(k) = 0. \tag{8.27}$$

Therefore, $\mathrm{supp}\tilde{\phi}$ is contained in

$$\{k \in \mathbb{R}^{1,3} \mid k^2 + m^2 = 0\}. \tag{8.28}$$

For $\vec{k} \in \mathbb{R}^3$, set $\varepsilon = \varepsilon(\vec{k}) := \sqrt{\vec{k}^2 + m^2}$. The set (8.28) consists of two hyperboloids, the positive frequency and negative frequency hyperboloid. $k \in \mathbb{R}^{1,3}$ from the positive frequency hyperboloid can be written as $k := (\varepsilon(\vec{k}), \vec{k})$. $k \in \mathbb{R}^{1,3}$ of this form will be called *on shell*. If we introduce "positive", resp. "negative frequency plane waves"

$$|k) = \frac{1}{\sqrt{(2\pi)^3}\sqrt{2\varepsilon(\vec{k})}}\mathrm{e}^{\mathrm{i}(-\varepsilon(\vec{k})x^0 + \vec{k}\vec{x})}, \tag{8.29}$$

$$|-k) = \overline{|k)} = \frac{1}{\sqrt{(2\pi)^3}\sqrt{2\varepsilon(\vec{k})}}\mathrm{e}^{-\mathrm{i}(-\varepsilon(\vec{k})x^0 + \vec{k}\vec{x})}, \tag{8.30}$$

then we can write

$$\phi(x) = \int \left(a^*(k)|k) + a(k)\overline{|k)}\right)\mathrm{d}\vec{k}, \tag{8.31}$$

which defines for k on shell, we define plane wave functionals $a(k)$, $a^*(k)$. Clearly, (8.31) can be rewritten as

$$\begin{aligned}\phi(x) &= \int \frac{\mathrm{d}\vec{k}}{\sqrt{(2\pi)^3}\sqrt{2\varepsilon(\vec{k})}}\left(\mathrm{e}^{\mathrm{i}kx}a(k) + \mathrm{e}^{-\mathrm{i}kx}a^*(k)\right),\\ \pi(x) &= \int \frac{\mathrm{d}\vec{k}\sqrt{\varepsilon(\vec{k})}}{\mathrm{i}\sqrt{(2\pi)^3}\sqrt{2}}\left(\mathrm{e}^{\mathrm{i}kx}a(k) - \mathrm{e}^{-\mathrm{i}kx}a^*(k)\right).\end{aligned}$$

After setting $x^0 = 0$, we can invert these relations:

$$a(k) = \int \frac{\mathrm{d}\vec{x}}{\sqrt{(2\pi)^3}}\mathrm{e}^{-\mathrm{i}\vec{k}\vec{x}}\left(\sqrt{\frac{\varepsilon(\vec{k})}{2}}\phi(0,\vec{x}) + \frac{\mathrm{i}}{\sqrt{2\varepsilon(\vec{k})}}\pi(0,\vec{x})\right), \tag{8.32}$$

$$a^*(k) = \int \frac{\mathrm{d}\vec{x}}{\sqrt{(2\pi)^3}}\mathrm{e}^{\mathrm{i}\vec{k}\vec{x}}\left(\sqrt{\frac{\varepsilon(\vec{k})}{2}}\phi(0,\vec{x}) - \frac{\mathrm{i}}{\sqrt{2\varepsilon(\vec{k})}}\pi(0,\vec{x})\right). \tag{8.33}$$

(8.48) can be rewritten with $\zeta_1, \zeta_2 \in \mathcal{Y}_{\mathrm{KG}}$ as

$$\omega(\zeta_1,\zeta_2) = -\mathrm{i}\int\left(\overline{\langle a(k)|\zeta_1\rangle}\langle a(k)|\zeta_2\rangle - \langle a(k)|\zeta_1\rangle\overline{\langle a(k)|\zeta_2\rangle}\right)\mathrm{d}\vec{k}. \tag{8.34}$$

Rewriting it in a shorter form we see that $a(k)$, $a^*(k)$ diagonalize the symplectic form:

$$\omega = -\mathrm{i}\int \mathrm{d}\vec{k}a^*(k)\wedge a(k). \tag{8.35}$$

They also diagonalize simultaneously the Hamiltonian and the momentum:

$$H = \int \mathrm{d}\vec{k}\varepsilon(\vec{k})a^*(k)a(k), \tag{8.36}$$

$$\vec{P} = \int \mathrm{d}\vec{k}\vec{k}a^*(k)a(k). \tag{8.37}$$

(8.35) is equivalent to

$$\{a(k),a(k')\} = \{a^*(k),a^*(k')\} = 0, \tag{8.38}$$

$$\{a(k),a^*(k')\} = -\mathrm{i}\delta(\vec{k}-\vec{k}'). \tag{8.39}$$

Hence,

$$\{a(k),H\} = -\mathrm{i}\varepsilon(\vec{k})a(k), \quad \{a^*(k),H\} = \mathrm{i}\varepsilon(\vec{k})a^*(k), \tag{8.40}$$

$$\{a(k),\vec{P}\} = -\mathrm{i}\vec{k}a(k), \quad \{a^*(k),\vec{P}\} = \mathrm{i}\vec{k}a^*(k), \tag{8.41}$$

8.5 Positive frequency space

Let us stress that the space $\mathcal{Y}_{\rm KG}$ is real, which reflects the fact that in this section we consider neutral fields. It is however useful to complexify the space $\mathcal{Y}_{\rm KG}$, that is to consider the space of smooth space-compact complex solutions of the Klein-Gordon equation. A possible notation for this space is $\mathbb{C}\mathcal{Y}_{\rm KG}$, but we will also use a different letter $\mathcal{W}_{\rm KG} := \mathbb{C}\mathcal{Y}_{\rm KG}$.

We multiply the current (8.10) by i and extend it by sesquilinearity to $\mathcal{W}_{\rm KG}$, obtaining

$$\mathrm{i}j^\mu(x,\overline{\zeta}_1,\zeta_2) \quad := \quad \mathrm{i}\big(\partial^\mu\overline{\zeta}_1(x)\zeta_2(x) - \overline{\zeta}_1(x)\partial^\mu\zeta_2(x)\big). \tag{8.42}$$

After integrating on a Cauchy surface we obtain the Hermitian form on $\mathcal{W}_{\rm KG}$:

$$\mathrm{i}\omega(\overline{\zeta}_1,\zeta_2) = \mathrm{i}\int \big(-\overline{\dot\zeta_1(t,\vec x)}\zeta_2(t,\vec x) + \overline{\zeta_1(t,\vec x)}\dot\zeta_2(t,\vec x)\big)\mathrm{d}\vec x. \tag{8.43}$$

We also extend by sesquilinearity to $\mathcal{W}_{\rm KG}$ the Hamiltonian and the momentum:

$$\langle H|\zeta\rangle = \frac{1}{2}\int \big(|\dot\zeta(t,\vec x)|^2 + |\vec\nabla\zeta(t,\vec x)|^2 + m^2|\zeta(t,\vec x)|^2\big)\mathrm{d}\vec x, \tag{8.44}$$

$$\langle P_j|\zeta\rangle = -\frac{1}{2}\int \big(\overline{\dot\zeta(t,\vec x)}\nabla_j\zeta(t,\vec x) + \overline{\nabla_j\zeta(t,\vec x)}\dot\zeta(t,\vec x)\big)\mathrm{d}\vec x. \tag{8.45}$$

Every $\zeta \in \mathcal{W}_{\rm KG}$ can be written in a unique way as

$$\zeta = \zeta^{(+)} + \zeta^{(-)}, \tag{8.46}$$

where $\zeta^{(\pm)}(k)$ are wave packets made of (8.29) and (8.30), and they do not have to be conjugate to one another:

$$\zeta^{(\pm)}(x) \quad = \quad \int \zeta^{(\pm)}(k)|\pm k)\mathrm{d}\vec k. \tag{8.47}$$

We obtain

$$\mathrm{i}\omega(\overline{\zeta_1},\zeta_2) = \int \overline{\zeta_1^{(+)}(k)}\zeta_2^{(+)}(k)\mathrm{d}\vec k - \int \overline{\zeta_1^{(-)}}(k)\zeta_2^{(-)}(k)\mathrm{d}\vec k \tag{8.48}$$

$$\langle H|\zeta\rangle = \frac{1}{2}\int \varepsilon(\vec k)\big(\overline{\zeta^{(+)}(k)}\zeta^{(+)}(k) + \overline{\zeta^{(-)}(k)}\zeta^{(-)}(k)\big)\mathrm{d}\vec k \tag{8.49}$$

$$\langle P^i|\zeta\rangle = \frac{1}{2}\int k^i\big(\overline{\zeta^{(+)}(k)}\zeta^{(+)}(k) + \overline{\zeta^{(-)}(k)}\zeta^{(-)}(k)\big)\mathrm{d}\vec k. \tag{8.50}$$

(8.46) gives a decomposition of the space $\mathbb{C}\mathcal{Y}_{\rm KG}$ into two subspaces

$$\mathbb{C}\mathcal{Y}_{\rm KG} = \mathcal{W}^{(+)}_{\rm KG} \oplus \mathcal{W}^{(-)}_{\rm KG}. \tag{8.51}$$

(8.48) restricted to $\mathcal{W}^{(+)}_{\rm KG}$ is positive definite. For $\zeta_1^{(+)},\zeta_2^{(+)} \in \mathcal{W}^{(+)}$ we will write

$$(\zeta_1^{(+)}|\zeta_2^{(+)}) := \mathrm{i}\overline{\zeta_1^{(+)}}\omega\zeta_2^{(+)}. \tag{8.52}$$

The *Hilbert space of positive energy solutions* is denoted $\mathcal{Z}^{(+)}_{\rm KG}$, and is the completion of $\mathcal{W}^{(+)}_{\rm KG}$ in this scalar product. $\mathcal{Z}^{(+)}_{\rm KG}$ can be identified with $L^2(\mathbb{R}^3)$, (8.52) rewritten as

$$(\zeta^{(+)}_1|\zeta^{(+)}_2) \quad = \quad \int \overline{\zeta^{(+)}(k)}\zeta^{(+)}(k)\mathrm{d}\vec{k}. \tag{8.53}$$

and $\zeta^{(+)}(k) = (k|\zeta^{(+)})$.

In this section we will not use $\mathcal{W}^{(-)}_{\rm KG}$ for quantization, however we will do this when we consider charged fields. Anticipating our discussion of charged fields of the next section, we introduce the space complex conjugate to $\mathcal{W}^{(-)}_{\rm KG}$, denoted $\overline{\mathcal{W}^{(-)}_{\rm KG}}$ and equipped with the scalar product

$$(\overline{\zeta}^{(-)}_1|\overline{\zeta}^{(-)}_2) \quad := \quad \mathrm{i}\zeta^{(-)}_1\omega\overline{\zeta^{(-)}_2}. \tag{8.54}$$

We set $\mathcal{Z}^{(-)}_{\rm KG}$ to be the completion of $\overline{\mathcal{W}^{(-)}_{\rm KG}}$ in this scalar product. (The bar is again the complex conjugation). $\mathcal{Z}^{(-)}_{\rm KG}$ can be identified with $L^2(\mathbb{R}^3)$ and (8.54) rewritten as

$$(\overline{\zeta}^{(-)}_1|\overline{\zeta}^{(-)}_2) \quad = \quad \int \zeta^{(-)}_1(k)\overline{\zeta^{(-)}_2(k)}\mathrm{d}\vec{k}$$

and $\overline{\zeta^{(-)}(k)} = \overline{(-k|}\overline{\zeta}^{(-)})$.

Note that $\overline{\mathcal{W}^{(-)}_{\rm KG}} = \mathcal{W}^{(+)}_{\rm KG}$, where we use the usual (internal) complex conjugation in $\mathcal{W}_{\rm KG}$. Therefore in principle we could identify $\mathcal{Z}^{(-)}_{\rm KG}$ and $\mathcal{Z}^{(+)}_{\rm KG}$. In particular, with this identification

$$\overline{|-k)} = |k). \tag{8.55}$$

This identification is consistently applied in this section, however in the next section we treat $\mathcal{Z}^{(-)}_{\rm KG}$ and $\mathcal{Z}^{(+)}_{\rm KG}$ as two separate Hilbert spaces.

$\mathbb{R}^{1,3} \rtimes O^{\uparrow}(1,3)$ acts on $\mathcal{Z}^{(+)}_{\rm KG}$ and $\mathcal{Z}^{(-)}_{\rm KG}$ in a natural way.

We have a natural identification of $\mathcal{Y}_{\rm KG}$ with $\mathcal{W}^{(+)}_{\rm KG}$. Indeed, $\zeta \in \mathcal{Y}_{\rm KG}$ can be projected onto $\zeta^{(+)} \in \mathcal{W}^{(+)}_{\rm KG}$, as in (8.46).This identification allows us to define a real scalar product on $\mathcal{Y}_{\rm KG}$:

$$\langle\zeta_1|\zeta_2\rangle_{\mathcal{Y}} \quad := \quad \mathrm{Re}(\zeta^{(+)}_1|\zeta^{(+)}_2).$$

We can compute explicitly this scalar product:

$$\begin{aligned}\langle\zeta_1|\zeta_2\rangle_{\mathcal{Y}} \quad &= \quad \int\int \dot{\zeta}_1(0,\vec{x})G^{(+)}(0,\vec{x}-\vec{y})\dot{\zeta}_2(0,\vec{y})\mathrm{d}\vec{x}\mathrm{d}\vec{y} \\ &\quad + \int\int \zeta_1(0,\vec{x})(-\Delta_{\vec{x}}+m^2)G^{(+)}(0,\vec{x}-\vec{y})\zeta_2(0,\vec{y})\mathrm{d}\vec{x}\mathrm{d}\vec{y}.\end{aligned} \tag{8.56}$$

8.6 Quantization of scalar fields

There are several equivalent presentations of free scalar quantum fields.

The description in typical physics textbooks can be described more or less as follows. We want to construct $\mathcal{H}, \hat{H}, \Omega$ such that H is a positive self-adjoint operator on $\mathcal{H}$, Ω is a normalized eigenvector of H with eigenvalue 0 and a self-adjoint operator valued distribution

$$\mathbb{R}^{1,3} \ni x \mapsto \hat{\phi}(x), \tag{8.57}$$

such that, with $\hat{\pi}(x) := \dot{\hat{\phi}}(x)$,

(1) $(-\Box + m^2)\hat{\phi}(x) = 0$,

(2) $[\hat{\phi}(0,\vec{x}), \hat{\phi}(0,\vec{y})] = [\hat{\pi}(0,\vec{x}), \hat{\pi}(0,\vec{y})] = 0$,
$[\hat{\phi}(0,\vec{x}), \hat{\pi}(0,\vec{y})] = \mathrm{i}\delta(\vec{x}-\vec{y})$.

(3) $\mathrm{e}^{\mathrm{i}t\hat{H}}\hat{\phi}(x^0,\vec{x})\mathrm{e}^{-\mathrm{i}t\hat{H}} = \hat{\phi}(x^0+t,\vec{x})$.

(4) Ω is cyclic for $\hat{\phi}(x)$.

Let us describe quantum scalar fields following the above strategy, as an (essentially unique) solution of the above problem. Let $\mathbb{R}^{1,3} \ni x \mapsto \hat{\phi}(x), \hat{\pi}(x)$ satisfy (1). Then the Fourier transform of $\hat{\phi}$ has to be supported on the mass hyperboloid. Therefore, by the same argument as in the classical case we can introduce $\hat{a}^*(k)$ and $\hat{a}(k)$ such that

$$\hat{\phi}(x) = \int \frac{\mathrm{d}\vec{k}}{\sqrt{(2\pi)^3}\sqrt{2\varepsilon(\vec{k})}} \left(\mathrm{e}^{\mathrm{i}kx}\hat{a}(k) + \mathrm{e}^{-\mathrm{i}kx}\hat{a}^*(k)\right), \tag{8.58}$$

$$\hat{\pi}(x) = \int \frac{\mathrm{d}\vec{k}\sqrt{\varepsilon(\vec{k})}}{\mathrm{i}\sqrt{(2\pi)^3}\sqrt{2}} \left(\mathrm{e}^{\mathrm{i}kx}\hat{a}(k) - \mathrm{e}^{-\mathrm{i}kx}\hat{a}^*(k)\right), \tag{8.59}$$

with the inverse transformation

$$\hat{a}(k) = \int \frac{\mathrm{d}\vec{x}}{\sqrt{(2\pi)^3}}\mathrm{e}^{-\mathrm{i}\vec{k}\vec{x}}\left(\sqrt{\frac{\varepsilon(\vec{k})}{2}}\phi(0,\vec{x}) + \frac{\mathrm{i}}{\sqrt{2\varepsilon(\vec{k})}}\pi(0,\vec{x})\right), \tag{8.60}$$

$$\hat{a}^*(k) = \int \frac{\mathrm{d}\vec{x}}{\sqrt{(2\pi)^3}}\mathrm{e}^{\mathrm{i}\vec{k}\vec{x}}\left(\sqrt{\frac{\varepsilon(\vec{k})}{2}}\hat{\phi}(0,\vec{x}) - \frac{\mathrm{i}}{\sqrt{2\varepsilon(\vec{k})}}\hat{\pi}(0,\vec{x})\right). \tag{8.61}$$

(These are identities (8.32) and (8.33) decorated with hats). Again, repeating the classical arguments, (2) implies

$$[\hat{a}(k), \hat{a}(k')] = [\hat{a}^*(k), \hat{a}^*(k')] = 0, \tag{8.62}$$

$$[\hat{a}(k), \hat{a}^*(k')] = \delta(\vec{k}-\vec{k}'). \tag{8.63}$$

We still need the Hilbert space and the Hamiltonian. Since we have an infinite number of degrees of freedom we cannot use the symmetric quantization

to define $\hat{H}$, because this would produce an infinite constant. Differentiating (3) wrt time we obtain

$$\mathrm{i}[\hat{H}, \hat{\phi}(x)] = \hat{\pi}(x). \tag{8.64}$$

This is equivalent to

$$[\hat{a}(k), \hat{H}] = \varepsilon(\vec{k})\hat{a}(k), \quad [\hat{a}^*(k), \hat{H}] = -\varepsilon(\vec{k})a^*(k), \tag{8.65}$$

$\hat{H}\Omega = 0$ implies $\hat{H}\hat{a}(k)\Omega = -\varepsilon(\vec{k})\hat{a}(k)\Omega$. But $\hat{H} \geq 0$. Thus we should assume

$$\hat{a}(k)\Omega = 0. \tag{8.66}$$

By (4), Ω is cyclic for $\hat{a}(k)$ and $\hat{a}^*(k)$. Using the commutation relations and (8.66) we see that Ω is cyclic just for $\hat{a}^*(k)$. In other words, $\mathcal{H}$ is spanned by vectors of the form

$$\Psi = \int \Psi(\vec{k}_1, \ldots, \vec{k}_n)\hat{a}^*(k_1) \cdots \hat{a}^*(k_n)\Omega \mathrm{d}\vec{k}_1 \cdots \mathrm{d}\vec{k}_n.$$

From the commutation relations and (8.66) we obtain

$$(\Psi|\Psi') = n! \int \overline{\Psi(\vec{k}_1, \ldots, \vec{k}_n)}\Psi'(\vec{k}_1, \ldots, \vec{k}_n)\mathrm{d}\vec{k}_1 \cdots \mathrm{d}\vec{k}_n.$$

This is exactly the scalar product for $\Gamma_{\mathrm{s}}(L^2(\mathbb{R}^3))$.

Besides the Hamiltonian $\hat{H}$ satisfying (8.65), we also want the momentum operator $\vec{\hat{P}}$, which satisfies

$$[\hat{a}(k), \vec{\hat{P}}] = \vec{k}\hat{a}(k), \qquad [\hat{a}^*(k), \vec{\hat{P}}] = -\vec{k}\hat{a}^*(k). \tag{8.67}$$

This fixes $\hat{H}$ and $\vec{\hat{P}}$ up to a constant. We choose the normal ordered form for these operators, which guarantees that they annihilate Ω:

$$\begin{aligned} \hat{H} &:= \int \hat{a}^*(k)\hat{a}(k)\varepsilon(\vec{k})\mathrm{d}\vec{k}, \\ \vec{\hat{P}} &:= \int \hat{a}^*(k)\hat{a}(k)\vec{k}\mathrm{d}\vec{k}. \end{aligned}$$

Recall that $L^2(\mathbb{R}^3)$ coincides with $\mathcal{Z}_{\mathrm{KG}}$, the completion of $\mathcal{W}^{(+)}_{\mathrm{KG}}$. Thus the Hilbert space $\mathcal{H}$ can be identified with $\Gamma_{\mathrm{s}}\big(\mathcal{Z}_{\mathrm{KG}}\big)$, Ω with the Fock vacuum, $\hat{a}^*(k)$ with the creation operators in the "physicist's notation".

As usual, we can also introduce the smeared versions of (8.60), (8.61) for $f \in \mathcal{Z}_{\mathrm{KG}}$:

$$\hat{a}(f) = \int \overline{f(k)}\hat{a}(k)\mathrm{d}\vec{k}; \tag{8.68}$$

$$\hat{a}^*(f) = \int f(k)\hat{a}^*(k)\mathrm{d}\vec{k}; \tag{8.69}$$

$$[\hat{a}(f), \hat{a}(f')] = [\hat{a}^*(f), \hat{a}^*(f')] = 0, \quad [\hat{a}(f), \hat{a}^*(f')] = (f|f'). \tag{8.70}$$

Using the "smeared notation" on the right we can write

$$\hat{a}^*(k) \quad = \quad \hat{a}^*\big(|k)\big). \tag{8.71}$$

The group $\mathbb{R}^{1,3} \rtimes O^\uparrow(1,3)$ acts on $\mathcal{W}^{(+)}_{\mathrm{KG}}$, and hence on $\mathcal{Z}_{\mathrm{KG}}$ by unitary transformations $r_{(y,\Lambda)}\Big|_{\mathcal{Z}_{\mathrm{KG}}}$. It acts unitarily also on $\Gamma_{\mathrm{s}}(\mathcal{Z}_{\mathrm{KG}})$ by $U(y,\Lambda) := \Gamma\Big(r_{(y,\Lambda)}\Big|_{\mathcal{Z}_{\mathrm{KG}}}\Big)$. On classical fields the Poincare group acts by $\phi(\Lambda x + y)$, see (8.9). On quantum fields the analog of this action is unitarily implemented:

$$U(y,\Lambda)\hat{\phi}(x)U(y,\Lambda)^* = \hat{\phi}\big((y,\Lambda)x\big).$$

This is true even though we only required that time translations are implemented.

One of possible alternative presentations of quantization of the free scalar field in the mathematical style goes as follows. We have the symplectic space $(\mathcal{Y}_{\mathrm{KG}}, \omega)$. This symplectic space is equipped with a symplectic dynamics r_t generated by a positive classical Hamiltonian H. We would like to find a CCR representation

$$\mathcal{Y}_{\mathrm{KG}} \ni \zeta \mapsto W(\zeta) \in U(\mathcal{H}) \tag{8.72}$$

We want the quantum Hamiltonian $\hat{H}$ to be positive and compatible with the classical Hamiltonian, so that

$$W(r_t(\zeta)) = \mathrm{e}^{\mathrm{i}t\hat{H}} W(\zeta) \mathrm{e}^{-\mathrm{i}t\hat{H}}. \tag{8.73}$$

All of this is realized by the method of a positive energy representations, as described in Subsection 7.10.

8.7 Two-point functions

Introduce the time-ordering operations for space-time dependent operators:

$$\mathrm{T}\big(A(x)B(y)\big) = \theta(x^0 - y^0)A(x)B(y) + \theta(y^0 - x^0)B(y)A(x), \tag{8.74}$$

$$\overline{\mathrm{T}}\big(A(x)B(y)\big) = \theta(y^0 - x^0)A(x)B(y) + \theta(x^0 - y^0)B(y)A(x). \tag{8.75}$$

Note the identities

$$[\hat{\phi}(x), \hat{\phi}(y)] \quad = \quad -\mathrm{i}G^{\mathrm{PJ}}(x-y)\mathbb{1}, \tag{8.76a}$$

$$(\Omega|\hat{\phi}(x)\hat{\phi}(y)\Omega) \quad = \quad G^{(+)}(x-y), \tag{8.76b}$$

$$(\Omega|\mathrm{T}(\hat{\phi}(x)\hat{\phi}(y))\Omega) \quad = \quad -\mathrm{i}G^{\mathrm{F}}(x-y), \tag{8.76c}$$

$$(\Omega|\overline{\mathrm{T}}(\hat{\phi}(x)\hat{\phi}(y))\Omega) \quad = \quad \mathrm{i}G^{\overline{\mathrm{F}}}(x-y). \tag{8.76d}$$

In fact,

$$\begin{aligned}
(\Omega|\hat{\phi}(x)\hat{\phi}(y)\Omega) &= \int\int \frac{\mathrm{d}\vec{k}\mathrm{d}\vec{k}'}{(2\pi)^3\sqrt{2\varepsilon}\sqrt{2\varepsilon'}}\mathrm{e}^{\mathrm{i}kx-\mathrm{i}k'y}(\Omega|\hat{a}(k)\hat{a}^*(k')\Omega) \\
&= \int \frac{\mathrm{d}\vec{k}}{(2\pi)^3 2\varepsilon(\vec{k})}\mathrm{e}^{\mathrm{i}k(x-y)} \\
&= G^{(+)}(x-y); \\
(\Omega|\mathrm{T}(\hat{\phi}(x)\hat{\phi}(y))\Omega) &= \theta(x^0-y^0)(\Omega|\hat{\phi}(x)\hat{\phi}(y)\Omega) + \theta(y^0-x^0)(\Omega|\hat{\phi}(y)\hat{\phi}(x)\Omega) \\
&= \theta(x^0-y^0)G^{(+)}(x-y) + \theta(y^0-x^0)G^{(-)}(x-y) \\
&= -\mathrm{i}G^{\mathrm{F}}(x-y),
\end{aligned}$$

where at the end we used (4.19).

Differentiating if needed (8.76b) with respect time we obtain the equal time correlation functions expressed as real symmetric kernels:

$$(\Omega|\hat{\phi}(0,\vec{x})\hat{\phi}(0,\vec{y})\Omega) = G^{(+)}(0,\vec{x}-\vec{y}), \tag{8.77}$$

$$(\Omega|\hat{\phi}(0,\vec{x})\hat{\pi}(0,\vec{y})\Omega) = 0, \tag{8.78}$$

$$\begin{aligned}
(\Omega|\hat{\pi}(0,\vec{x})\hat{\pi}(0,\vec{y})\Omega) &= -\partial_t^2 G^{(+)}(0,\vec{x}-\vec{y}) \\
&= (-\Delta_{\vec{x}}+m^2)G^{(+)}(0,\vec{x}-\vec{y}).
\end{aligned} \tag{8.79}$$

8.8 Spacetime smeared fields

For $f \in C_{\mathrm{c}}^{\infty}(\mathbb{R}^{1,3},\mathbb{R})$ set

$$\hat{\phi}[f] := \int f(x)\hat{\phi}(x)\mathrm{d}x. \tag{8.80}$$

The operators $\hat{\phi}[f]$ are essentially self-adjoint for $f \in C_{\mathrm{c}}^{\infty}(\mathcal{O},\mathbb{R})$ on, say, smooth vectors in the Fock space with compact supports. Therefore, we can define $W(f) := \mathrm{e}^{\mathrm{i}\hat{\phi}[f]}$.

We have

$$[\hat{\phi}[f],\hat{\phi}[g]] = -\mathrm{i}\int\int f(x)g(x)G^{\mathrm{PJ}}(x-y)\mathrm{d}y\mathrm{d}y. \tag{8.81}$$

In particular, if $\mathrm{supp}(f)\times\mathrm{supp}(g)$, then $\hat{\phi}[f]$ and $\hat{\phi}[g]$ commute.

(8.76b) implies the following identities for spacetime smeared fields and Weyl operators:

$$(\Omega|\hat{\phi}[f]^2\Omega) = \int\int f(x)G^{(+)}(x-y)f(y)\mathrm{d}x\mathrm{d}y, \tag{8.82}$$

$$(\Omega|\mathrm{e}^{\mathrm{i}\hat{\phi}[f]}\Omega) = \exp\left(-\frac{1}{2}\int\int f(x)G^{(+)}(x-y)f(y)\mathrm{d}x\mathrm{d}y\right). \tag{8.83}$$

(8.80) satisfy the Wightman axioms with $\mathcal{D} := \Gamma_{\mathrm{s}}^{\mathrm{fin}}(\mathcal{Z}_{\mathrm{KG}})$.

For an open set $\mathcal{O} \subset \mathbb{R}^d$ we set

$$\mathfrak{A}(\mathcal{O}) := \{\exp(\mathrm{i}\hat{\phi}[f]) \ : \ f \in C_{\mathrm{c}}^{\infty}(\mathcal{O}, \mathbb{R})\}''.$$

The algebras $\mathfrak{A}(\mathcal{O})$ satisfy the Haag-Kastler axioms.

8.9 Physical meaning of the 2-point functions and Feynman propagators

Let us now describe Gedankenexperiments measuring the 2-point function and the Feynman propagator.

First let us note a general fact. Suppose that we are able to create a state $\Phi \in \mathcal{H}$, $\|\Phi\| = 1$. On the measurement side, let us select two non-parallel vectors $\Psi_i \in \mathcal{H}$, $i = 1, 2$. Suppose for any i, j we can measure

$$A_i := |\Psi_i)(\Psi_i| + |\Psi_i)(\Psi_i|, \quad i = 1, 2, \tag{8.84}$$

$$B := |\Psi_1)(\Psi_2| + |\Psi_2)(\Psi_1|, \quad C := \mathrm{i}|\Psi_1)(\Psi_2| - \mathrm{i}|\Psi_2)(\Psi_1|. \tag{8.85}$$

Measuring A_i we obtain $(\Phi|A_i\Phi) = |(\Phi|\Psi_i)|^2$, $i = 1, 2$. Measuring B, C, we can determine $\frac{(\Phi|\Psi_1)}{(\Phi|\Psi_2)}$. Thus from these measurements we can determine the amplitudes $(\Psi_i|\Phi)$, $i = 1, 2$ up to an overall phase factor.

Gedankenexperiment 1. Let us choose spacetime functions f, g_i. Suppose we prepare the state given by $\Phi := \hat{\phi}[f]\Omega$. We can assume that it is normalized. Set $\Psi_i := \hat{\phi}[g_i]\Omega$. Then up to an overall phase factor we are able to measure the amplitudes

$$(\Psi_i|\Phi) = \int (\Omega|\hat{\phi}(y)\hat{\phi}(x)\Omega) g_i(y) f(x) \mathrm{d}x \mathrm{d}y, \tag{8.86}$$

which can be expressed in terms of the 2-point function.

Gedankenexperiment 2. Suppose now that we can perturb the dynamics by adding to the Lagrangian $-\lambda f(x)\phi(x)$. Then the interaction Hamiltonian becomes

$$\hat{H}_{\mathrm{Int}}(t) = \lambda \int f(t, \vec{x}) \hat{\phi}(t, \vec{x}) \mathrm{d}\vec{x}, \tag{8.87}$$

where $\hat{\phi}(x)$ are the free fields. Suppose we measure the vaccum–vacuum amplitude. The resulting quantity is

$$\Big(\Omega|\mathrm{T}\exp\Big(-\mathrm{i}\int \hat{H}_{\mathrm{Int}}(t)\mathrm{d}t\Big)\Omega\Big) \tag{8.88}$$

$$= \sum_{n=0}^{\infty} (-\mathrm{i})^n \int_{t_n > \cdots > t_1} \cdots \int (\Omega|\hat{H}_{\mathrm{Int}}(t_n) \cdots \hat{H}_{\mathrm{Int}}(t_1)\Omega) \mathrm{d}t_n \cdots \mathrm{d}t_1 \tag{8.89}$$

$$= \exp\Big(-\frac{\lambda^2}{2} \int \int f(x) f(y) (\Omega|\mathrm{T}\{\hat{\phi}(x)\hat{\phi}(y)\}\Omega) \mathrm{d}x \mathrm{d}y\Big), \tag{8.90}$$

which is expressed in terms of the Feynman propagator.

Note that the second scenario is probably more realistic. Thus one can argue that the Feynman propagator is more physical than the 2-point function.

9 Free charged scalar bosons

The formalism used in physics to describe complex fields, and especially to quantize them, is different from the real case, therefore we devote to it a separate section.

9.1 Lagrangian formalism

Consider the space of complex smooth functions on the spacetime $C^\infty(\mathbb{R}^{1,3}) = C^\infty(\mathbb{R}^{1,3},\mathbb{C})$. Clearly, the space $C^\infty(\mathbb{R}^{1,3})$ is equipped with a *complex conjugation* $f \mapsto \overline{f}$ and a $U(1)$ *symmetry* $f \mapsto \mathrm{e}^{\mathrm{i}\theta} f$, $\theta \in \mathbb{R}/2\pi\mathbb{Z} = U(1)$.

If T is a real linear functional on $C^\infty(\mathbb{R}^{1,3})$, then we have two kinds of natural complex conjugations of T:

$$\langle \overline{T}|\zeta\rangle := \overline{\langle T|\overline{\zeta}\rangle}, \qquad \langle T^*|\zeta\rangle := \overline{\langle T|\zeta\rangle}. \tag{9.1}$$

Both maps $T \mapsto \overline{T}$ and $T \mapsto T^*$ are antilinear. When restricted to the real subspace $\mathcal{Y}_{\mathrm{KG}} \subset C^\infty(\mathbb{R}^{1,3})$, the functionals $\overline{T}$ and T^* coincide. (Note that here $*$ does not denote the Hermitian conjugaton!)

A special role is played by *complex linear* functionals on $C^\infty(\mathbb{R}^{1,3})$. The space of such functionals will be denoted $C^\infty(\mathbb{R}^{1,3})^{\mathrm{T}}$. If $T \in C^\infty(\mathbb{R}^{1,3})^{\mathrm{T}}$, then $\overline{T} \in C^\infty(\mathbb{R}^{1,3})^{\mathrm{T}}$, unlike T^*, which is antilinear.

Let $\psi(x)$, $\psi^*(x)$ be the linear functionals on $C^\infty(\mathbb{R}^{1,3})$

$$\langle \psi(x)|f\rangle := f(x), \qquad \langle \psi^*(x)|f\rangle := \overline{f(x)}.$$

If $\mathcal{L}(x)$ is a Lagrangian density, which is a function of x, $\psi(x)$, $\psi^*(x)$, $\psi_{,\mu}(x)$ and $\psi^*_{,\mu}(x)$, then the Euler-Lagrange equations read

$$\partial_{\psi^*}\mathcal{L} - \partial_\mu \frac{\partial \mathcal{L}}{\partial \psi^*_{,\mu}} = 0, \tag{9.2}$$

$$\partial_{\psi}\mathcal{L} - \partial_\mu \frac{\partial \mathcal{L}}{\partial \psi_{,\mu}} = 0. \tag{9.3}$$

If $\mathcal{L}(x)$ is real, then (9.2) implies (9.3).

We consider the Lagrangian density

$$\mathcal{L}(x) = -\partial_\mu \psi^*(x)\partial^\mu \psi(x) - m^2 \psi^*(x)\psi(x). \tag{9.4}$$

Then the Euler-Lagrange equations are equivalent to the (complex) Klein-Gordon equation:

$$(-\Box + m^2)\psi(x) = 0. \tag{9.5}$$

The *variables conjugate* to $\psi(x)$ and $\psi^*(x)$ are

$$\begin{aligned} \eta^*(x) &:= \frac{\partial \mathcal{L}}{\partial \psi_{,0}(x)} = \partial_0 \psi^*(x), \\ \eta(x) &:= \frac{\partial \mathcal{L}}{\partial \psi^*_{,0}(x)} = \partial_0 \psi(x). \end{aligned}$$

$\mathcal{W}_{\rm KG}$ will denote the space of *smooth space-compact complex solutions of the Klein-Gordon equation*

$$(-\Box + m^2)\zeta = 0. \tag{9.6}$$

(In the context of neutral fields, it was denoted $\mathbb{C}\mathcal{Y}_{\rm KG}$, because it was an auxiliary object, the *complexification of the phase space* $\mathcal{Y}_{\rm KG}$. Now it is the basic object, the *phase space* itself). In the on-shell formalism we will consider $\psi(x)$, $\psi^*(x)$, $\eta^*(x)$ and $\eta(x)$ as functionals on $\mathcal{W}_{\rm KG}$.

(8.6) implies

$$\psi(t,\vec{x}) = \int \dot{G}^{\rm PJ}(t,\vec{x}-\vec{y})\psi(0,\vec{y})\mathrm{d}\vec{y} + \int G^{\rm PJ}(t,\vec{x}-\vec{y})\eta(0,\vec{y})\mathrm{d}\vec{y}. \tag{9.7}$$

9.2 Charged fields as a pair of neutral fields

Let us go back to the Lagrangian formalism. For $x \in \mathbb{R}^{1,3}$ let us introduce the fields $\phi_{\rm R}(x)$, $\phi_{\rm I}(x)$ as the functionals on $C^\infty(\mathbb{R}^{1,3})$ given by

$$\langle \phi_{\rm R}(x)|f\rangle := \sqrt{2}{\rm Re}f(x), \qquad \langle \phi_{\rm I}(x)|f\rangle := \sqrt{2}{\rm Im}f(x). \tag{9.8}$$

or equivalently

$$\psi(x) = \frac{1}{\sqrt{2}}\big(\phi_{\rm R}(x) + {\rm i}\phi_{\rm I}(x)\big), \quad \psi^*(x) = \frac{1}{\sqrt{2}}\big(\phi_{\rm R}(x) - {\rm i}\phi_{\rm I}(x)\big).$$

Clearly, the Lagrangian density can be rewritten as

$$\mathcal{L}(x) = -\frac{1}{2}\partial_\mu\phi_{\rm R}(x)\partial^\mu\phi_{\rm R}(x) - \frac{1}{2}m^2\phi_{\rm R}(x)^2 \tag{9.9}$$

$$-\frac{1}{2}\partial_\mu\phi_{\rm I}(x)\partial^\mu\phi_{\rm I}(x) - \frac{1}{2}m^2\phi_{\rm I}(x)^2. \tag{9.10}$$

The usual real formalism yields a pair of neutral fields with the usual equal time Poisson brackets (we write only the non-vanishing ones):

$$\{\phi_{\rm R}(t,\vec{x}),\pi_{\rm R}(t,\vec{y})\} = \{\phi_{\rm I}(t,\vec{x}),\pi_{\rm I}(t,\vec{y})\} \quad = \quad \delta(\vec{x}-\vec{y}). \tag{9.11}$$

The fields with an additional symmetry

$$\phi^\theta_{\rm R} = \cos\theta\phi_{\rm R} - \sin\theta\phi_{\rm I}, \tag{9.12}$$

$$\phi^\theta_{\rm I} = \sin\theta\phi_{\rm R} + \cos\theta\phi_{\rm I}. \tag{9.13}$$

The equal-time Poisson brackets, which follow from (9.11) are

$$\{\psi(t,\vec{x}),\eta^*(t,\vec{y})\} = \{\psi^*(t,\vec{x}),\eta(t,\vec{y})\} \quad = \quad \delta(\vec{x}-\vec{y}). \tag{9.14}$$

(We write only non-vanishing ones). Using (9.7) we obtain

$$\begin{aligned}\{\psi(x),\psi(y)\} = \{\psi^*(x),\psi^*(y)\} &= 0,\\ \{\psi(x),\psi^*(y)\} &= -G^{\rm PJ}(x-y).\end{aligned}$$

9.3 Classical 4-current

The Lagrangian is invariant w.r.t. the $U(1)$ symmetry $\psi \mapsto \mathrm{e}^{-\mathrm{i}\theta}\psi$. The Noether 4-current associated to this symmetry is called simply the *4-current*. It is

$$\begin{aligned}\mathcal{J}^\mu(x) &:= \mathrm{i}\Big(\psi^*(x)\frac{\partial\mathcal{L}(x)}{\partial\psi^*_{,\mu}} - \frac{\partial\mathcal{L}(x)}{\partial\psi_{,\mu}}\psi(x)\Big)\\ &= \mathrm{i}\big(\partial^\mu\psi^*(x)\psi(x) - \psi^*(x)\partial^\mu\psi(x)\big).\end{aligned}$$

It is conserved on shell and real:

$$\begin{aligned}\partial_\mu\mathcal{J}^\mu(x) &= 0,\\ \mathcal{J}^\mu(x)^* &= \mathcal{J}^\mu(x).\end{aligned}$$

Up to a coefficient, it coincides with the current (8.42) evaluated at $\zeta = \zeta_1 = \zeta_2$.

$$\begin{aligned}\langle\mathcal{J}^\mu(x)|\zeta\rangle &= \mathrm{i}j^\mu(\overline{\zeta},\zeta,x)\\ &= \mathrm{i}\big(\overline{\partial^\mu\zeta(x)}\zeta(x) - \overline{\zeta(x)}\partial^\mu\zeta(x)\big).\end{aligned}$$

The 0th component of the 4-current is called the *charge density*

$$\mathcal{Q}(x) := \mathcal{J}^0(x) = \mathrm{i}\big(-\eta^*(x)\psi(x) + \psi^*(x)\eta(x)\big).$$

We have the relations

$$\begin{aligned}\{\mathcal{Q}(t,\vec{x}),\psi(t,\vec{y})\} &= \mathrm{i}\psi(t,\vec{y})\delta(\vec{x}-\vec{y}),\\ \{\mathcal{Q}(t,\vec{x}),\eta(t,\vec{y})\} &= \mathrm{i}\eta(t,\vec{y})\delta(\vec{x}-\vec{y}),\\ \{\mathcal{Q}(t,\vec{x}),\mathcal{Q}(t,\vec{y})\} &= 0.\end{aligned} \tag{9.15}$$

The *(total) charge*

$$Q := \int \mathcal{Q}(t,\vec{x})\mathrm{d}\vec{x}$$

is conserved (does not depend on time) and coincides with the quadratic form obtained from (8.43):

$$\langle Q|\zeta\rangle = \mathrm{i}\overline{\zeta}\omega\zeta. \tag{9.16}$$

9.4 Stress-energy tensor

The Lagrangian is invariant w.r.t. space-time translations. This leads to the *stress-energy tensor*

$$\begin{aligned}\mathcal{T}^{\mu\nu}(x) &:= -\frac{\partial\mathcal{L}(x)}{\partial\psi_{,\mu}(x)}\partial^\nu\psi(x) - \partial^\nu\psi^*(x)\frac{\partial\mathcal{L}(x)}{\partial\psi^*_{,\mu}(x)} + g^{\mu\nu}\mathcal{L}(x)\\ &= \partial^\mu\psi^*(x)\partial^\nu\psi(x) + \partial^\nu\psi^*(x)\partial^\mu\psi(x)\\ &\quad -g^{\mu\nu}\left(\partial_\alpha\psi^*(x)\partial^\alpha\psi(x) + m^2\psi^*(x)\psi(x)\right).\end{aligned}$$

It is conserved on shell

$$\partial_\mu\mathcal{T}^{\mu\nu}(x) = 0.$$

The components of the stress-energy tensor with the first temporal coordinate are called the Hamiltonian density and momentum density. We express them on-shell in terms of $\psi(x)$, $\psi^*(x)$, $\eta(x)$ and $\eta^*(x)$:

$$\begin{aligned}\mathcal{H}(x) &:= \mathcal{T}^{00}(x) &&= \eta^*(x)\eta(x) + \vec{\partial}\psi^*(x)\vec{\partial}\psi(x) + m^2\psi^*(x)\psi(x),\\ \mathcal{P}^i(x) &:= \mathcal{T}^{0i}(x) &&= -\eta^*(x)\partial^i\psi(x) - \partial^i\psi^*(x)\eta(x).\end{aligned}$$

$\mathcal{H}(x)$ and $\vec{\mathcal{P}}(x)$ acting on $\zeta \in \mathcal{W}_{\mathrm{KG}}$ yield

$$\begin{aligned}\langle \mathcal{H}(x)|\zeta\rangle &= |\dot{\zeta}(x)|^2 + |\vec{\partial}\zeta(x)|^2 + m^2|\zeta(x)|^2,\\ \langle \vec{\mathcal{P}}(x)|\zeta\rangle &= -\overline{\dot{\zeta}(x)}\vec{\partial}\zeta(x) - \overline{\vec{\partial}\zeta(x)}\dot{\zeta}(x).\end{aligned}$$

We easily check

$$\{\psi(t,\vec{x}), \mathcal{H}(t,\vec{y})\} = \dot{\psi}(t,\vec{x})\delta(\vec{x}-\vec{y}), \tag{9.17}$$
$$\{\eta(t,\vec{x}), \mathcal{H}(t,\vec{y})\} = \dot{\eta}(t,\vec{x})\delta(\vec{x}-\vec{y}), \tag{9.18}$$
$$\{\psi(t,\vec{x}), \mathcal{P}^i(t,\vec{y})\} = -\partial^i\psi(t,\vec{x})\delta(\vec{x}-\vec{y}), \tag{9.19}$$
$$\{\eta(t,\vec{x}), \mathcal{P}^i(t,\vec{y})\} = -\partial^i\eta(t,\vec{x})\delta(\vec{x}-\vec{y}). \tag{9.20}$$

We introduce the *(total) Hamiltonian* and *momentum*:

$$H := \int_{\mathcal{S}} \mathcal{T}^{\mu 0}(x)\mathrm{d}s_\mu(x) = \int \mathcal{H}(t,\vec{x})\mathrm{d}\vec{x}, \tag{9.21}$$
$$P^i := \int_{\mathcal{S}} \mathcal{T}^{\mu i}(x)\mathrm{d}s_\mu(x) = \int \mathcal{P}^i(t,\vec{x})\mathrm{d}\vec{x}. \tag{9.22}$$

where $\mathcal{S}$ is any Cauchy subspace.

H and $\vec{P}$ are the generators of the time and space translations:

$$\dot{\psi}(x) = \{\psi(x), H\}, \quad \dot{\eta}(x) = \{\eta(x), H\},$$
$$\vec{\partial}\psi(x) = -\{\psi(x), \vec{P}\}, \quad \vec{\partial}\eta(x) = -\{\eta(x), \vec{P}\}.$$

The observables H, P^1, P^2, P^3 and Q are in involution.

9.5 Simultaneous diagonalization

We have the following observables in involution:

$$\langle Q|\zeta\rangle = \mathrm{i}\int \big(-\overline{\dot{\zeta}(x)}\zeta(x) + \overline{\zeta(x)}\dot{\zeta}(x)\big)\mathrm{d}\vec{x}, \tag{9.23}$$
$$\langle H|\zeta\rangle = \int \big(|\dot{\zeta}(x)|^2 + |\vec{\nabla}\zeta(x)|^2 + m^2|\zeta(x)|^2\big)\mathrm{d}\vec{x}, \tag{9.24}$$
$$\langle P_j|\zeta\rangle = -\int \big(\overline{\dot{\zeta}(x)}\nabla_j\zeta(x) + \overline{\nabla_j\zeta(x)}\dot{\zeta}(x)\big)\mathrm{d}\vec{x}. \tag{9.25}$$

Note that (8.44) and (8.45) from the neutral case differ from (9.24) and (9.25) only by the prefactor $\frac{1}{2}$.

We use the Fourier transformation and (8.46):

$$\langle Q|\zeta\rangle = \int \big(\overline{\zeta^{(+)}}(k)\zeta^{(+)}(k)\mathrm{d}\vec{k} - \overline{\zeta^{(-)}}(k)\zeta^{(-)}(k)\big)\mathrm{d}\vec{k} \tag{9.26}$$

$$\langle H|\zeta\rangle = \int \varepsilon(\vec{k})\big(\overline{\zeta^{(+)}(k)}\zeta^{(+)}(k) + \overline{\zeta^{(-)}(k)}\zeta^{(-)}(k)\big)\mathrm{d}\vec{k} \tag{9.27}$$

$$\langle P^i|\zeta\rangle = \int k^i\big(\overline{\zeta^{(+)}(k)}\zeta^{(+)}(k) + \overline{\zeta^{(-)}(k)}\zeta^{(-)}(k)\big)\mathrm{d}\vec{k}. \tag{9.28}$$

9.6 Negative frequency space

Recall that for $\vec{k} \in \mathbb{R}^3$, set $\varepsilon = \varepsilon(\vec{k}) := \sqrt{\vec{k}^2 + m^2}$ and every $\zeta \in \mathcal{W}_{\mathrm{KG}}$ can be written in a unique way as

$$\zeta = \zeta^{(+)} + \zeta^{(-)}, \tag{9.29}$$

where

$$\zeta^{(\pm)}(x) \quad = \quad \int \zeta^{(\pm)}(k)\frac{1}{\sqrt{(2\pi)^3}\sqrt{2\varepsilon(\vec{k})}}\mathrm{e}^{\pm\mathrm{i}(-\varepsilon(\vec{k})x^0 + \vec{k}\vec{x})}\mathrm{d}\vec{k}. \tag{9.30}$$

(9.29) gives a decomposition of the space $\mathbb{C}\mathcal{Y}_{\mathrm{KG}}$ into two subspaces

$$\mathbb{C}\mathcal{Y}_{\mathrm{KG}} = \mathcal{W}^{(+)}_{\mathrm{KG}} \oplus \mathcal{W}^{(-)}_{\mathrm{KG}}. \tag{9.31}$$

We have already introduced the positive energy space $\mathcal{W}^{(+)}$ together with its completion $\mathcal{Z}^{(+)}$. We will also need the negative frequency space $\mathcal{W}^{(-)}_{\mathrm{KG}}$. Let c denote the complex conjugation on $\mathcal{W}^{(-)}_{\mathrm{KG}}$. We actually have two distinct interpretations of c: as the usual complex conjugation inside $\mathcal{W}$, so that $c : \mathcal{W}^{(-)}_{\mathrm{KG}} \to \mathcal{W}^{(+)}_{\mathrm{KG}}$ and In particular, $c|-k) = |k)$, or as the identity on $\mathcal{W}^{(-)}$, such that $c\mathrm{i} = -\mathrm{i}c$. We have the scalar product

$$(c\zeta^{(-)}_1|c\zeta^{(-)}_2) \quad := \quad \mathrm{i}\zeta^{(-)}_1\omega\overline{\zeta^{(-)}_2}. \tag{9.32}$$

We set $\mathcal{Z}^{(-)}_{\mathrm{KG}}$ to be the completion of $c\mathcal{W}^{(-)}_{\mathrm{KG}}$ in this scalar product. $\mathcal{Z}^{(-)}_{\mathrm{KG}}$ can be identified with $L^2(\mathbb{R}^3)$ and (9.32) rewritten as

$$(c\zeta^{(-)}_1|c\zeta^{(-)}_2) \quad = \quad \int \zeta^{(-)}_1(k)\overline{\zeta^{(-)}_2(k)}\mathrm{d}\vec{k}$$

$\mathbb{R}^{1,3} \rtimes O^{\uparrow}(1,3)$ acts on $\mathcal{Z}^{(+)}_{\mathrm{KG}}$ and $\mathcal{Z}^{(-)}_{\mathrm{KG}}$ in a natural way.

9.7 Plane wave functionals

Plane wave functionals are defined as linear or antilinear functionals on the complex space $\mathcal{W}_{\mathrm{KG}}$, for any $\zeta \in \mathcal{W}_{\mathrm{KG}}$ given by

$$\langle a(k)|\zeta\rangle = \zeta^{(+)}(k), \qquad \langle a^*(k)|\zeta\rangle = \overline{\zeta^{(+)}(k)} \tag{9.33}$$

$$\langle b(k)|\zeta\rangle = \overline{\zeta^{(-)}(k)} \qquad \langle b^*(k)|\zeta\rangle = \zeta^{(-)}(k). \tag{9.34}$$

Thus

$$\begin{aligned}
a(k) &= \int \Big(\sqrt{\frac{\varepsilon(\vec{p})}{2}}\psi(0,\vec{x}) + \frac{\mathrm{i}}{\sqrt{2\varepsilon(\vec{k})}}\eta(0,\vec{x})\Big)\mathrm{e}^{-\mathrm{i}\vec{k}\vec{x}}\frac{\mathrm{d}\vec{x}}{\sqrt{(2\pi)^3}},\\
a^*(k) &= \int \Big(\sqrt{\frac{\varepsilon(\vec{k})}{2}}\psi^*(0,\vec{x}) - \frac{\mathrm{i}}{\sqrt{2\varepsilon(\vec{k})}}\eta^*(0,\vec{x})\Big)\mathrm{e}^{\mathrm{i}\vec{k}\vec{x}}\frac{\mathrm{d}\vec{x}}{\sqrt{(2\pi)^3}},\\
b(k) &= \int \Big(\sqrt{\frac{\varepsilon(\vec{k})}{2}}\psi^*(0,\vec{x}) + \frac{\mathrm{i}}{\sqrt{2\varepsilon(\vec{k})}}\eta^*(0,\vec{x})\Big)\mathrm{e}^{-\mathrm{i}\vec{k}\vec{x}}\frac{\mathrm{d}\vec{x}}{\sqrt{(2\pi)^3}},\\
b^*(k) &= \int \Big(\sqrt{\frac{\varepsilon(\vec{k})}{2}}\psi(0,\vec{x}) - \frac{\mathrm{i}}{\sqrt{2\varepsilon(\vec{k})}}\eta(0,\vec{x})\Big)\mathrm{e}^{\mathrm{i}\vec{k}\vec{x}}\frac{\mathrm{d}\vec{x}}{\sqrt{(2\pi)^3}},
\end{aligned}$$

The only non-vanishing Poisson bracket are

$$\{a(k), a^*(k')\} = \{b(k), b^*(k')\} = -\mathrm{i}\delta(\vec{k}-\vec{k}').$$

We have the following expressions for the fields:

$$\begin{aligned}
\psi(x) &= \int \frac{\mathrm{d}\vec{k}}{\sqrt{(2\pi)^3}\sqrt{2\varepsilon(\vec{k})}}\left(\mathrm{e}^{\mathrm{i}kx}a(k) + \mathrm{e}^{-\mathrm{i}kx}b^*(k)\right),\\
\eta(x) &= \int \frac{\mathrm{d}\vec{k}\sqrt{\varepsilon(\vec{k})}}{\mathrm{i}\sqrt{(2\pi)^3}\sqrt{2}}\left(\mathrm{e}^{\mathrm{i}kx}a(k) - \mathrm{e}^{-\mathrm{i}kx}b^*(k)\right).
\end{aligned}$$

We have accomplished the diagonalization of the basic observables:

$$\begin{aligned}
H &= \int \mathrm{d}\vec{k}\varepsilon(\vec{k})\big(a^*(k)a(k) + b^*(k)b(k)\big),\\
\vec{P} &= \int \mathrm{d}\vec{k}\vec{k}\big(a^*(k)a(k) + b^*(k)b(k)\big),\\
Q &= \int \mathrm{d}\vec{k}\big(a^*(k)a(k) - b^*(k)b(k)\big).
\end{aligned}$$

As usual, for $f \in \mathcal{K}_{\mathrm{KG}}^{(+)}$, $g \in \mathcal{K}_{\mathrm{KG}}^{(-)}$, we have smeared versions of the above

functionals:

$$\langle a(f)|\zeta\rangle = \int \overline{f(k)}\zeta^{(+)}(k)\mathrm{d}\vec{k}, \qquad a(f) = \int \overline{f(k)}a(k)\mathrm{d}\vec{k}; \tag{9.35}$$

$$\langle a^*(f)|\zeta\rangle = \int f(k)\overline{\zeta^{(+)}(k)}\mathrm{d}\vec{k}, \qquad a^*(f) = \int f(k)a^*(k)\mathrm{d}\vec{k}; \tag{9.36}$$

$$\langle b(g)|\zeta\rangle = \int \overline{b(k)}\overline{\zeta^{(-)}(k)}\mathrm{d}\vec{k}, \qquad b(g) = \int \overline{g(k)}b(k)\mathrm{d}\vec{k}; \tag{9.37}$$

$$\langle b^*(g)|\zeta\rangle = \int g(k)\zeta^{(-)}(k)\mathrm{d}\vec{k}, \qquad b^*(g) = \int g(k)b^*(k)\mathrm{d}\vec{k}; \tag{9.38}$$

$$\{a(f), a^*(f')\} = -\mathrm{i}(f|f'); \qquad \{b(g), b^*(g')\} = -\mathrm{i}(g|g'). \tag{9.39}$$

Thus, for k on the mass shell, using physicist's notation on the left and mathematician's on the right, we can write

$$a^*(k) \;=\; a^*\big(|k)\big), \tag{9.40}$$

$$b^*(k) \;=\; b^*\big(c|-k)\big). \tag{9.41}$$

9.8 Quantization

In principle, we could quantize the complex Klein-Gordon equation as a pair of real Klein-Gordon fields. However, we will use the formalism of quantization of charged bosonic systems, see Subsect. 7.11.

We want to construct $(\mathcal{H}, \hat{H}, \Omega)$ satisfying the usual requirements of QM (1)-(3) and an operator valued distribution

$$\mathbb{R}^{1,3} \ni x \mapsto \hat{\psi}(x) \tag{9.42}$$

satisfying, with $\hat{\eta}(x) := \dot{\hat{\psi}}(x)$,

(1) $(-\Box + m^2)\hat{\psi}(x) = 0$;

(2) the only non-vanishing 0-time commutators are

$$[\hat{\psi}(0,\vec{x}), \hat{\eta}^*(0,\vec{y})] = \mathrm{i}\delta(\vec{x}-\vec{y}), \quad [\hat{\psi}^*(0,\vec{x}), \hat{\eta}(0,\vec{y})] = \mathrm{i}\delta(\vec{x}-\vec{y}); \tag{9.43}$$

(3) $\mathrm{e}^{\mathrm{i}t\hat{H}}\hat{\psi}(x^0,\vec{x})\mathrm{e}^{-\mathrm{i}t\hat{H}} = \hat{\psi}(x^0+t,\vec{x})$;

(4) Ω is cyclic for $\hat{\psi}(x)$, $\hat{\psi}^*(x)$.

The above problem has an essentially unique solution, which we describe below.

We set

$$\mathcal{H} := \Gamma_{\mathrm{s}}(\mathcal{Z}_{\mathrm{KG}}^{(+)} \oplus \mathcal{Z}_{\mathrm{KG}}^{(-)}).$$

Creation/annihilation operators for the particle space $\mathcal{Z}_{\mathrm{KG}}^{(+)} \simeq L^2(\mathbb{R}^3)$ are denoted with the letter a and for the antiparticle space $\mathcal{Z}_{\mathrm{KG}}^{(-)} \simeq L^2(\mathbb{R}^3)$ with the

letter b. Thus we put hats and do all the obvious modifications to the classical formulas. Ω is the Fock vacuum. The quantum field is

$$\begin{aligned}\hat{\psi}(x) &:= \int \frac{\mathrm{d}\vec{k}}{\sqrt{(2\pi)^3}\sqrt{2\varepsilon(\vec{k})}} \Big(\mathrm{e}^{\mathrm{i}px}\hat{a}(k) + \mathrm{e}^{-\mathrm{i}kx}\hat{b}^*(k)\Big),\\ \hat{\eta}(x) &:= \int \frac{\mathrm{d}\vec{k}\sqrt{\varepsilon(\vec{k})}}{\mathrm{i}\sqrt{(2\pi)^3}\sqrt{2}} \Big(\mathrm{e}^{\mathrm{i}kx}\hat{a}(k) - \mathrm{e}^{-\mathrm{i}kx}\hat{b}^*(k)\Big).\end{aligned}$$

The quantum Hamiltonian, momentum and charge are

$$\begin{aligned}\hat{H} &:= \int \Big(\hat{a}^*(k)\hat{a}(k) + \hat{b}^*(k)\hat{b}(k)\Big)\varepsilon(\vec{k})\mathrm{d}\vec{k}, \qquad (9.44)\\ \vec{\hat{P}} &:= \int \Big(\hat{a}^*(k)\hat{a}(k) + \hat{b}^*(k)\hat{b}(k)\Big)\vec{k}\mathrm{d}\vec{k},\\ \hat{Q} &:= \int \Big(\hat{a}^*(k)\hat{a}(k) - \hat{b}^*(k)\hat{b}(k)\Big)\mathrm{d}\vec{k}.\end{aligned}$$

Equivalently, for any t

$$\begin{aligned}\hat{H} &= \int :\Big(\hat{\eta}^*(t,\vec{x})\hat{\eta}(t,\vec{x}) + \vec{\partial}\hat{\psi}^*(t,\vec{x})\vec{\partial}\hat{\psi}(t,\vec{x}) + m^2\hat{\psi}^*(t,\vec{x})\hat{\psi}(t,\vec{x})\Big):\mathrm{d}\vec{x},\\ \vec{\hat{P}} &= \int :\Big(-\hat{\eta}^*(t,\vec{x})\vec{\partial}\hat{\psi}(t,\vec{x}) - \vec{\partial}\hat{\psi}^*(t,\vec{x})\hat{\eta}(t,\vec{x})\Big):\mathrm{d}\vec{x},\\ \hat{Q} &= \mathrm{i}\int :\Big(-\hat{\eta}^*(t,\vec{x})\hat{\psi}(t,\vec{x}) + \hat{\psi}^*(t,\vec{x})\hat{\eta}(t,\vec{x})\Big):\mathrm{d}\vec{x}.\end{aligned}$$

Thus all these operators are expressed in terms of the Wick quantization of their classical expressions.

Note that the whole group $\mathbb{R}^{1,3} \rtimes O^\uparrow(1,3)$ acts unitarily on $\mathcal{H}$ by $U(y,\Lambda) := \Gamma\Big(r_{(y,\Lambda)}\Big|_{\mathcal{Z}^{(+)}_{\mathrm{KG}}}\Big) \otimes \Gamma\Big(\overline{r}_{(y,\Lambda)}\Big|_{\mathcal{Z}^{(-)}_{\mathrm{KG}}}\Big)$, with

$$U(y,\Lambda)\hat{\psi}(x)U(y,\Lambda)^* = \hat{\psi}\big((y,\Lambda)x\big).$$

Moreover,

$$[\hat{\psi}(x),\hat{\psi}^*(y)] = -\mathrm{i}G^{\mathrm{PJ}}(x-y), \quad [\hat{\psi}(x),\hat{\psi}(y)] = 0.$$

Note the identities for the 2-point functions:

$$[\hat{\psi}(x),\hat{\psi}^*(y)] = -\mathrm{i}G^{\mathrm{PJ}}(x-y)\mathbb{1}, \qquad (9.45a)$$

$$(\Omega|\hat{\psi}(x)\hat{\psi}^*(y)\Omega) = G^{(+)}(x-y), \qquad (9.45b)$$

$$(\Omega|\hat{\psi}^*(x)\hat{\psi}(y)\Omega) = G^{(-)}(x-y), \qquad (9.45c)$$

$$(\Omega|\mathrm{T}(\hat{\psi}(x)\hat{\psi}^*(y))\Omega) = -\mathrm{i}G^{\mathrm{F}}(x-y), \qquad (9.45d)$$

$$(\Omega|\overline{\mathrm{T}}(\hat{\psi}(x)\hat{\psi}^*(y))\Omega) = \mathrm{i}G^{\overline{\mathrm{F}}}(x-y). \qquad (9.45e)$$

9.9 Smeared fields

For $f \in C_{\rm c}^\infty(\mathbb{R}^{1,3},\mathbb{C})$ we set

$$\hat\psi[f] := \int \overline{f(x)}\hat\psi(x)\mathrm{d}x, \qquad \hat\psi^*[f] := \int f(x)\hat\psi^*(x)\mathrm{d}x. \tag{9.46}$$

We obtain an operator valued distribution satisfying the Wightman axioms with $\mathcal{D} := \Gamma_{\rm s}^{\rm fin}(\mathcal{Z}_{\rm KG}^{(+)} \oplus \mathcal{Z}_{\rm KG}^{(-)})$.

For an open set $\mathcal{O} \subset \mathbb{R}^{1,3}$ the field algebra is defined as

$$\mathfrak{F}(\mathcal{O}) := \left\{ \exp\left(\mathrm{i}\hat\psi^*[f] + \mathrm{i}\hat\psi[f]\right) \ : \ f \in C_{\rm c}^\infty(\mathcal{O},\mathbb{C}) \right\}''.$$

The observable algebra $\mathfrak{A}(\mathcal{O})$ is the subalgebra of $\mathfrak{F}(\mathcal{O})$ fixed by the automorphism

$$B \mapsto \mathrm{e}^{\mathrm{i}\theta\hat Q} B \mathrm{e}^{-\mathrm{i}\theta\hat Q}.$$

The algebras $\mathfrak{F}(\mathcal{O})$ and $\mathfrak{A}(\mathcal{O})$ satisfy the *Haag-Kastler axioms*.

10 Some historical remarks on QFT

This section should be treated as a collection of gossips and loose statements. I will discuss only quantum field theory in its traditional sense such as QED or Standard Model. Various more modern constructions that grew out of Quantum Field Theory, such as String Theory, 2-dimensional Conformal Theories, topological field theories, Chern-Simons Theory, supersymmetric theories, etc, are outside of the scope of these remarks.

In this section I will consider both bosons and fermions. Bosons will be denoted ϕ and fermions ψ.

10.1 Physicist's strategy in QFT

Here is an outline of the usual physicist's strategy. It was essentially developed by Feynman, Schwinger, Tomonaga and Dyson in the late 40's.

1. Start with free fields. They are given by quantizing the following Lagrangians:

$$\mathcal{L}(x) = -\frac{1}{2}\partial_\mu\phi(x)\partial^\mu\phi(x) - \frac{m^2}{2}\phi^2(x) \quad \text{for bosons,} \tag{10.1}$$

$$\mathcal{L}(x) = \mathrm{i}\overline{\psi}(x)\gamma_\mu\partial^\mu\psi(x) + m\overline{\psi}(x)\psi(x), \quad \text{for fermions.} \tag{10.2}$$

2. Add a perturbation local in fields. Typical perturbations include $\lambda\phi(x)^4$, Yukawa $\lambda\phi(x)\overline{\psi}(x)\psi(x)$. Often these perturbations are obtained by the minimal coupling prescription and lead to a gauge theory. Usually one assumes that the perturbation is Lorentz invariant, even in fermions, and the resulting Hamiltonian is positive.

3. Compute formally the perturbation expansion of the scattering operator between in states Φ_- and out states Φ_+:

$$\lim_{t\to\infty}(\Phi_+|\mathrm{e}^{\mathrm{i}tH_0}\mathrm{e}^{-\mathrm{i}2tH_\lambda}\mathrm{e}^{\mathrm{i}tH_0}\Phi_-) = (\Phi_+|S(\lambda)\Phi_-) \tag{10.3}$$

$$= \sum_{n=0}^{\infty} \lambda^n (\Phi_+|S_n\Phi_-), \tag{10.4}$$

   expressing it in Feynman diagrams.

4. The terms S_n given by the above prescriptions are ill defined in many ways. Give them a meaning by renormalization, which leads to a well-defined formal series expressing scattering amplitudes.

5. From scattering amplitudes compute scattering cross-sections of physical processes.

10.2 Renormalizability

Consider the Lagrangian of the form (10.1) or (10.2) in d spacetime dimensions. We want the action to be scalar and the kinetic term to have no dimensionful coefficient. This implies that in the units of length the boson field has the dimension $[\phi] = 1 - \frac{d}{2}$ and the fermion field the dimension $[\psi] = \frac{1}{2} - \frac{d}{2}$. Clearly $\deg \partial = -1$.

The full Lagrangian is typically the sum of monomials in fields. The action integral should be dimensionless. The integral includes the Lebesgue measure $\mathrm{d}^d x$, which has dimension d. Therefore, if the dimension of a monomial is c, then one has to put a coupling constant in front of dimension $-d - c$.

We will say that a monomial is

1. *super-renormalizable* if the corresponding coupling constant has a negative dimension.

2. *marginally* or *just renormalizable* if it has a dimensionless coupling constant.

3. *non-renormalizable* if it has a coupling constant of a positive dimension.

Super-renormalizable and marginally renormalizable terms are joiuntly called *renormalizable*. One can show that in renormalizable theories one needs only a finite number of parameters to fix renormalization conditions. In super-renormalizable theories it is enough to renormalize Feynman diagrams up to a certain finite order—in marginally renormalizable theories one has to do it in any order (but still the number of parameters is finite).

In the old days, physicists used to believe that physical theories should be renormalizable. Nowadays physicists view non-renormalizable Lagrangians as useful tools for the description of the matter as well. The dominant view says that all known quantum field theories that we use are only *effective*, and their

validity is limited to low energies. Therefore, one should not treat them as ultimate theories.

Nevertheless, renormalizable theories are distinguished. In fact, they have clearly a better predictive power than non-renormalizable theories. There are also well-known arguments attributed to Kenneth Wilson, involving the change of scale, often called the renormalization group, which explain a different role of renormalizable and non-renormalizable terms in the Lagrangian.

Let us review the renormalizability of various monomials in the Lagrangian in various dimensions.

- **d=2.** $\deg\phi = 0, \quad \deg\psi = -\frac{1}{2}$.

$$\begin{aligned} \text{super-renormalizable} \qquad & P(\phi), \quad P(\phi)\partial\phi \quad P(\phi)\overline{\psi}\psi; \\ \text{marginally renormalizable} \qquad & P(\phi)(\overline{\psi}\psi)^2, \quad P(\phi)\overline{\psi}\partial\psi, \quad P(\phi)(\partial\phi)^2. \end{aligned}$$

- **d=3.** $\deg\phi = -\frac{1}{2}, \quad \deg\psi = -1$.

$$\begin{aligned} \text{super-renormalizable} \qquad & \phi^3, \phi^4, \phi^5, \phi^2\partial\phi, \quad \phi\overline{\psi}\psi; \\ \text{marginally renormalizable} \qquad & \phi^6, \phi^3\partial\phi, \quad \phi^2\overline{\psi}\psi. \end{aligned}$$

- **d=4.** $\deg\phi = -1, \quad \deg\psi = -\frac{3}{2}$.

$$\begin{aligned} \text{super-renormalizable} \qquad & \phi^3; \\ \text{marginally renormalizable} \qquad & \phi^4, \phi^2\partial\phi, \quad \phi\overline{\psi}\psi. \end{aligned}$$

- **d=6.** $\deg\phi = -2, \quad \deg\psi = -\frac{5}{2}$.

$$\text{marginally renormalizable} \qquad \phi^3.$$

ϕ, ϕ^2, $\partial\phi$, $\phi\partial\phi$ and $\overline{\psi}\psi$ are always super-renormalizable (this includes the mass terms).

$(\partial\phi)^2$ and $\overline{\psi}\partial\psi$ are always marginally renormalizable (this includes the kinetic terms).

10.3 Counterterms

Let us consider for instance the $\lambda\phi_4^4$ theory. Naive computations based on the Lagrangian

$$\mathcal{L}(x) = -\frac{1}{2}\partial_\mu\phi(x)\partial^\mu\phi(x) - \frac{m^2}{2}\phi^2(x) - \lambda\phi(x)^4 \tag{10.5}$$

lead to ill-defined quantities. In order to obtain sensible predictions one has to consider the Lagrangian involving counterterms, which is traditionally written

as

$$\mathcal{L}(x) = -Z\Big(\frac{1}{2}\partial_\mu\phi(x)\partial^\mu\phi(x) + \frac{m^2}{2}\phi^2(x)\Big) - Z^2 g\phi(x)^4 \tag{10.6}$$

$$Z = \sum_{n=0}^{\infty} Z_n\lambda^n, \qquad Z_0 = 1; \tag{10.7}$$

$$m = \sum_{n=0}^{\infty} m_n\lambda^n, \qquad m_0 = m; \tag{10.8}$$

$$g = \sum_{n=1}^{\infty} g_n\lambda^n, \qquad g_1 = 1. \tag{10.9}$$

Then one recursively computes the time-ordered N-point correlation function

$$G(x_N, \dots, x_1) := \Big(\Omega|\big(\mathrm{T}\big(\phi(x_N)\cdots\phi(x_1)\big)\Omega\Big).$$

Usually one introduces some regularization depending on a parameter Λ (a cut-off, Pauli-Villars, dimensional, etc.). Regularized quantities are finite, and then one takes the limit $\Lambda \to \infty$. It is also possible to avoid the use of a regularization (this is the case of the BPHZ method, and also the Epstein-Glaser method). All these schemes give the same answers, which depend on 3 parameters.

There are various ways to fix these parameters. Typically, one imposes the "mass shell condition" on $G(p)$, the Fourier transform of the 2-point function:

$$G(p) \approx (p^2 + m^2)^{-1}, \quad p^2 \approx -m^2. \tag{10.10}$$

One needs also a condition on the 4-point function.

From the time-ordered N-point functions the LSZ formulas lead to scattering amplitudes (matrix elements of the scattering operator).

The situation is different in the massless case. The mass-shell condition cannot be usually applied. Besides, scattering amplitudes are ill defined because of the infra-red problem. Instead, one can compute inclusive cross-sections.

Let us replace ϕ^4 with ϕ^n for $n > 4$. This perturbation is non-renormalizable. There exist solutions of the recursive procedure indicated above, however in order to fix them one needs an infinite number of parameters.

10.4 Asymptotic freedom

Some classes of Feynman diagrams can be summed up. For instance, when computing the 2-point function for interacting photon in QED using the geometric series, one can sum up diagrams that consist of repeated 1-particle irreducible terms. One obtains

$$G(k) = \frac{1}{1 - \Sigma(k)} G_0(k). \tag{10.11}$$

The quantity $\Sigma(k)$, usually called the self-energy, can be computed in the lowest order. One obtains a function that grows for large k. Therefore, at least in

this approximation, there is a pole for large energies and it is clear that (10.11) becomes worthless. Its discovery is attributed to Landau, and the corresponding pole is called the *Landau pole*. The same phenomenon can be seen for most other QFT's, such as $\lambda\phi^4$.

There exists a version of the above argument based on the renormalization group equation that also predicts the existence of a pole in these theories and is even more convincing.

Landau, after discovering the pole named after him, announced the death of Quantum Field Theory. In reality, if the coupling constant is very small, the pole is very far in high energies and one can ignore it in perturbative calculations—this is the case of QED. However, when the coupling constant is not so small, problems related to the Landau pole may appear close to physical energies. This is the case of the Standard Model, where there is a ϕ^4 term in the Higgs field.

Quantization of the Yang-Mills theory is much more difficult than that of fields with an Abelian gauge or no local gauge at all. Nevertheless, by the early 70's it was well understood and it was proven by t'Hooft and Veltman that the gauge invariance survives renormalization. In the Yang-Mills theory instead of photons we have gluons. Gluons interact with themeselves, therefore in the gluon self-energy beside fermion loops we have (bosonic) gluon loops. They change the sign of the self-energy, and therefore (if there are not too many fermions) there is no Landau pole in the ultraviolet and the gluon propagator becomes suppressed for large energies. This property of the Yang-Mills theory is called asymptotic freedom. It was discovered in the early 70's. It implies that the Yang-Mills theory can be applied in large energies. This lead in the 70's to an enthusiastic revival of QFT.

Apparently, t'Hooft did first the computation proving the asymptotic freedom of the Yang-Mills theory, but did not recognize its physical importance. The asymptotic freedom of Yang-Mills was shown (simultaneously?) by Gross-Wilczek and Politzer. For many years they were on the list of candidates for the Nobel Prize, until eventually they got it.

10.5 Axiomatic Quantum Field Theory

Axiomatic Quantum Field Theory tries to derive theorems starting from axioms, such as the Wightman and Haag-Kastler axioms. Here are some of its early successes:

- The existence of the CPT transformation (in the framework of Wightman axioms).
- The link between spin and statistics (in the framework of Wightman axioms).
- The Haag-Ruelle scattering theory—construction of the scattering matrix starting from Haag-Kastler axioms with a discrete mass shell.
- The Doplicher-Haag-Roberts theory—description of superselection sectors and their relationship to global gauge groups.

Another current of mathematical research has been devoted to perturbative Quantum Field Theory. There is good understanding of renormalization of quantum fields, and also on a curved background.

10.6 Constructive Field Theory

Essentially all computations in Quantum Field Theory are perturbative around one of free theories. Free theories are not very interesting, because they have a trivial scattering operator. It is natural to ask whether there exist models of Quantum Field Theory other than free theories. This question was posed by Wightman, who formulated the set of axioms called nowadays after him. He proposed to try to construct interacting models satisfying these axioms.

It is natural to expect that mathematically constructible theories should be renormalizable. Wightman proposed to start constructions from the simplest, theories, in 1+1 dimensions, going up the ladder of difficulty, so that eventually one will be able to construct physically relevant models, expected to be difficult.

This program was initiated in the late 60's. Probably the most famous team in this program was that of James Glimm and Arthur Jaffe. They started with constructing the least complicated of the models from the list in Subsect. 10.2, that is $P(\phi)_2$. To define this model in a finite volume one only needs to Wick order the interaction and to subtract a divergent constant from the Hamiltonian. It took several papers and ingenious ideas before this model was fully constructed and all axioms were verified. An especially successful method turned out to be the Euclidean approach, which starts from a classical model on a Euclidean space with a local interaction and then applies the Wick rotation.

A similar successful construction has been accomplished for the Yukawa model in 2 dimensions, $\phi\overline{\psi}\psi_2$, and for $\lambda\phi^4_3$. These models are much more difficult and they require more complicated renormalization. Still, they are quite far from physical interest. In particular, they are super-renormalizable and live in dimension < 4.

A major problem with more physical models such as QED_4 and $\lambda\phi^4_4$ was the Landau pole, which essentially means that they are not likely to be constructed, at least using the perturbative strategy. This problem seems to be absent in the YM_4. A Polish mathematician Tadeusz Bałaban wrote a series of extremely difficult papers where he studied YM_4 in a finite volume. He considered Euclidean YM_4 on a lattice and apparently proved that the partition function is bounded away from zero uniformly in the lattice spacing. YM_4 on continuous Euclidean spacetime, also in a finite volume, was studied by Rivasseau, Magnen and Seneor by different methods. Both Bałaban and Rivasseau et al. claim that the ultraviolet problem of in a finite volume can be controlled. Neither has written a proof of this.

To my knowledge there exists one marginally renormalizable model that has been constructed: the Gross-Neveu model in dimension 2 with the Lagrangian

$$\overline{\psi}_a(\mathrm{i}\gamma^\mu\partial_\mu - m)\psi^a + \frac{g^2}{2N}(\overline{\psi}_a\psi^a)^2. \tag{10.12}$$

(N is the number of fermion species. For $N = 1$ the model reduces to the completely integrable Thirring model). It was constructed by Gawedzki–Kupiainen, and by Rivasseau et al.

In the early 90's the interest in constructive field theory waned and essentially this topic was abandoned by researchers. One reason for the collapse of the topic was that it became prohibitively complicated. Another reason was the philosophy proclaimed by Wilson saying that quantum field theories that we know are probably only low-energy effective approximations and one should not be surprised if they cannot be expressed in a mathematically satisfactory way.

Nowadays it is even very difficult to determine what has been proven and what are the proofs—the old literature is mostly unreadable. I know only one recent result in some kind of constructive field theory. Unfotunately, it is negative: Aizenman and Duminil-Copin proved that the $\lambda\phi_4^4$ theory is trivial. More precisely, if one tries to approximate it on a lattice, then in the limit one obtains a trivial theory.

At the turn of millenium the Clay Institute funded prizes of 1 milion dollars each for proving 7 important mathematical conjectures. One of them was proven (The Poincare Conjecturé by Grigorii Perelman, who declined the prize). Other are still open, including two conjectures in mathematical physics.

One of them is the existence of solutions to the Navier–Stokes equation. The problem is clearly formulated (by Charles Fefferman).

The other is the construction of the Yang-Mills Theory and the proof of the existence of a positive mass gap, (formulated by Arthur Jaffe and Edward Witten).

To my understanding, the formulation of the problem is vague. The description of the problem mentions Wightman axioms, however they seem not suitable for gauge theories. What is worse, even if we construct something that the Prize Committee will accept as the quantized Yang-Mills Theory, we have to prove the positivity of the mass gap (which involves controlling not only ultraviolet divergencies, but also the large volume limit). In other words, we need to show that the lightest glueball is massive—which is supposed to be the expression of the confinement.

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11 Time-dependent Hamiltonians

11.1 Schrödinger and Heisenberg picture

Suppose that H is a (time-independent) Hamiltonian. It generates the dynamics $\mathrm{e}^{-\mathrm{i}tH}$ on the Hilbert space $\mathcal{H}$. If we prepare a state ρ at time 0 and measure an observable A at time $t > 0$, then the expectation value of the measurement is

$$\mathrm{Tr}\rho\mathrm{e}^{\mathrm{i}tH}A\mathrm{e}^{-\mathrm{i}tH}. \tag{11.1}$$

In quantum physics two equivalent ways of expressing (11.1) are used:

(1) *The Schrödinger picture*: We let the state evolve $\rho(t) := \mathrm{e}^{-\mathrm{i}tH}\rho\mathrm{e}^{\mathrm{i}tH}$ and keep the observable constant. Then (11.1) equals $\mathrm{Tr}\rho(t)A$.

(2) *The Heisenberg picture*: We let the observable evolve $A(t) := \mathrm{e}^{\mathrm{i}tH}A\mathrm{e}^{-\mathrm{i}tH}$ and keep the state constant. Then (11.1) equals $\mathrm{Tr}\rho A(t)$.

(By the *Schrödinger picture* one also means the unitary evolution $\Psi(t) := \mathrm{e}^{-\mathrm{i}tH}\Psi$ on $\mathcal{H}$.)

11.2 Time-ordered exponential

We will often use the formalism of time-dependent Hamiltonians. In this subsection we describe the main concepts of this formalism.

Let $t \mapsto B_n(t), \ldots, B_1(t)$ be time dependent operators. Let $t_n, \ldots, t_1$ be pairwise distinct. We define the *time-ordered product of* $B_n(t_n)$,..., $B_1(t_1)$ by

$$\mathrm{T}\left(B_n(t_n)\cdots B_1(t_1)\right) := B_{\sigma_n}(t_{\sigma_n})\cdots B_{\sigma_1}(t_{\sigma_1}),$$

where $(\sigma_1, \ldots, \sigma_n)$ is the permutation such that $t_{\sigma_n} \geq \cdots \geq t_{\sigma_1}$.

Consider a family of self-adjoint operators

$$t \mapsto H(t). \tag{11.2}$$

For $t_+ > t_-$, we define the *time-ordered exponential*

$$\begin{aligned} &\mathrm{Texp}\left(-\mathrm{i}\int_{t_-}^{t_+} H(t)\mathrm{d}t\right) \qquad (11.3)\\ :=\ &\sum_{n=0}^{\infty}(-\mathrm{i})^n \int\cdots\int_{t_+\geq t_n\geq\cdots\geq t_1\geq t_-} H(t_n)\cdots H(t_1)\mathrm{d}t_n\cdots\mathrm{d}t_1\\ =\ &\sum_{n=0}^{\infty}(-\mathrm{i})^n \int_{t_-}^{t_+}\cdots\int_{t_-}^{t_+}\frac{1}{n!}\mathrm{T}\left(H(t_n)\cdots H(t_1)\right)\mathrm{d}t_n\cdots\mathrm{d}t_1. \end{aligned}$$

For brevity, we will write $U(t_+, t_-)$ for (11.3) and call it the *dynamics generated by* $t \mapsto H(t)$. Note that $U(t_+, t_-)$ are unitary. (The above constructions can be easily made rigorous if $H(t)$ are bounded. If they are unbounded, the above definition should be viewed only as a heuristic indication how to define the family of unitary operators $U(t_+, t_-)$. In most of this subsection we are not very precise about the boundedness of operators, types of limits, etc.)

We also set $U(t_-, t_+) := U(t_+, t_-)^{-1}$. Thus $U(t_+, t_-)$ is the solution of the following two equivalent equations:

$$\frac{\mathrm{d}}{\mathrm{d}t_+}U(t_+, t_-) = -\mathrm{i}H(t_+)U(t_+, t_-), \quad U(t, t) = \mathbb{1}; \tag{11.4}$$

$$\text{equivalently,} \quad \frac{\mathrm{d}}{\mathrm{d}t_-}U(t_+, t_-) = U(t_+, t_-)\mathrm{i}H(t_-), \quad U(t, t) = \mathbb{1}. \tag{11.5}$$

Clearly, if $H(t) = H$ does not depend on time, then $U(t_+, t_-) = \mathrm{e}^{-\mathrm{i}(t_+ - t_-)H}$.

We also have

$$U(t_+,t_-)=\lim_{n\to\infty}\prod_{j=1}^{n}\exp\Big(-\frac{\mathrm{i}(t_+-t_-)}{n}H\Big(\frac{jt_++(n-j)t_-}{n}\Big)\Big),\qquad(11.6)$$

where in the product the indices increase from the right to the left:

$$\prod_{j=1}^{n}A_j:=A_n\cdots A_1.\qquad(11.7)$$

11.3 Schrödinger and Heisenberg picture for time-dependent Hamiltonians

The formalism of the Schrödinger and Heisenberg picture described for time-independent Hamiltonians in Subsection 11.1 is somewhat more complicated if the Hamiltonian is time-dependent. Then the Hamiltonian in the Schrödinger picture and the Hamiltonian in the Heisenberg picture can be different.

Let us assume that the evolution $U(t_+,t_-)$ defined as in (11.3) corresponds to the Schrödinger picture, that is the evolution of vector states is

$$\Psi_{t_+}=U(t_+,t_-)\Psi_{t_-}.\qquad(11.8)$$

Thus the family of self-adjoint operators (11.2) can be called the *Hamiltonian in the Schrödinger picture*. Hence the evolution of a density matrix ρ in the *Schrödinger picture* from time 0 to time t is

$$\rho(t)=U(t,0)\rho U(0,t),\qquad(11.9)$$

and satisfies the equation

$$\frac{\mathrm{d}}{\mathrm{d}t}\rho(t)=-\mathrm{i}\left[H(t),\rho(t)\right],\qquad(11.10)$$

$$\rho(0)=\rho.\qquad(11.11)$$

Let us introduce the evolution of an observable A in the *Heisenberg picture*:

$$A(t):=U(0,t)AU(t,0),\qquad(11.12)$$

where we treat $t=0$ as the reference time. We then have two ways to express the time evolution of the expectation value:

$$\mathrm{Tr}\rho(t)A=\mathrm{Tr}\rho A(t).\qquad(11.13)$$

Equivalently, $A(t)$ is the solution of

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}A(t)&=\mathrm{i}\left[H^{\mathrm{Hp}}(t),A(t)\right],\qquad(11.14)\\ A(0)&=A,\end{aligned}$$

where the *Hamiltonian in the Heisenberg picture* is defined as

$$t \mapsto H^{\mathrm{Hp}}(t) := U(0,t)H(t)U(t,0). \tag{11.15}$$

Thus a quantum dynamics is described by two time-dependent Hamiltonians: $t \mapsto H(t)$ and $t \mapsto H^{\mathrm{Hp}}(t)$. If they do not depend on time, they coincide.

The dynamics can be obtained as a solution of equations similar to (11.4) and (11.5), involving the Hamiltonian in the Heisenberg picture. However, one of the times has to be the reference time (in our case 0), and the Hamiltonian appears "on the wrong side":

$$\frac{\mathrm{d}}{\mathrm{d}t}U(t,0) = -U(t,0)\mathrm{i}H^{\mathrm{Hp}}(t); \tag{11.16}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}U(0,t) = \mathrm{i}H^{\mathrm{Hp}}(t)U(0,t). \tag{11.17}$$

Thus we can compare:

$$U(t,0) = \mathrm{Texp}\left(-\mathrm{i}\int_0^t H(s)\mathrm{d}s\right), \tag{11.18}$$

$$U(t,0)^{-1} = U(0,t) = \mathrm{Texp}\left(\mathrm{i}\int_0^t H^{\mathrm{Hp}}(s)\mathrm{d}s\right). \tag{11.19}$$

11.4 Classical dynamics

To define an evolution on a classical phase space $\mathbb{R}^d$ we need to fix a vector field

$$\mathbb{R}\times\mathbb{R}^d \ni (t,x) \mapsto X(t,x) \in \mathbb{R}^d \tag{11.20}$$

The equation

$$\frac{\mathrm{d}}{\mathrm{d}t}x(t) = X\big(t,x(t)\big). \tag{11.21}$$

for any initial condition $x(0) = x_0 \in \mathbb{R}^d$, we obtain a solution $\mathbb{R} \ni t \mapsto x(t,x_0)$. This defines a flow $R(t,0)$on $\mathbb{R}^d$ such that $R(t,0)x_0 = x(t,x_0)$ and (11.22) can be rewritten as

$$\frac{\mathrm{d}}{\mathrm{d}t}R(t,0)x_0 = X\big(t,R(t,0)x_0\big). \tag{11.22}$$

In classical mechanics the phase space is described by coordinates $(\phi,\pi) \in \mathbb{R}^m \times \mathbb{R}^m$ with the Poisson bracket

$$\begin{aligned}\{\phi^i,\phi^j\} = \{\pi_i,\pi_j\} &= 0,\\ \{\phi^i,\pi_j\} &= \delta^i_j.\end{aligned}$$

The time evolution is described by a Hamiltonian

$$\mathbb{R}\times\mathbb{R}^{2m} \ni (t,\phi,\pi) \mapsto H(t,\phi,\pi) \in \mathbb{R}, \tag{11.23}$$

and the Hamilton equations

$$\begin{aligned} \dot{\phi}(t) &= \{\phi(t), H(t)\} \\ \dot{\pi}(t) &= \{\pi(t), H(t)\}. \end{aligned} \tag{11.24}$$

Note that the classical evolution equations (11.22) and (11.24) are analogs of the quantum equations in the Heisenberg picture (11.14). In particular, the classical Hamiltonian (11.23) is the analog of the quantum Hamiltonian in the Heisenberg picture (11.15).

There exists also a dual picture, which is the analog of the Schrödinger picture of Quantum Mechanics. Consider the evolution given by the backward flow. The analog of the equation (11.22) is

$$\frac{\mathrm{d}}{\mathrm{d}t} R(0,t)x_0 = -X^{\mathrm{Sp}}\big(t, R(0,t)x_0\big), \tag{11.25}$$

where

$$X^{\mathrm{Sp}}(t,y) = R'(0,t)X\big(t, R(t,0)y\big). \tag{11.26}$$

Thus the vector field is minus the backward transport of the original field. $R'(0,t)$ is the derivative of the flow.

In the Hamiltonian case we have the dynamics

$$\big(\phi^{\mathrm{Sp}}(t), \pi^{\mathrm{Sp}}(t)\big) = R(0,t)\big(\phi, \pi\big). \tag{11.27}$$

The map $R(0,t)$ is symplectic, therefore the Hamiltonian equation is transported to a Hamiltonian equation, however for a different Hamiltonian:

$$H^{\mathrm{Sp}}(t, \phi, \pi) = H\big(t, R(t,0)(\phi, \pi)\big). \tag{11.28}$$

More precisely, there is also the change of the sign:

$$\begin{aligned} \dot{\phi}^{\mathrm{Sp}}(t) &= -\{\phi^{\mathrm{Sp}}(t), H^{\mathrm{Sp}}(t)\} \\ \dot{\pi}^{\mathrm{Sp}}(t) &= -\{\pi^{\mathrm{Sp}}(t), H^{\mathrm{Sp}}(t)\}. \end{aligned} \tag{11.29}$$

Thus the classical and the quantum cases are analogous. However, whereas in the quantum case the Schrödinger picture seems preferred, in the classical case the analog of the Heisenberg picture seems to be more common. Therefore, in the quantum case we put the superscript Hp but not Sp, and the other way around in the classical case.

11.5 Time-dependent perturbations

Our time-dependent Hamiltonians will usually have the form

$$H(t) := H_{\mathrm{fr}} + \lambda V(t),$$

where H_{fr} is a self-adjoint operator and $\mathbb{R} \ni t \mapsto V(t)$ is a family of self-adjoint operators.

We can introduce the so-called *interaction picture* or the *Furry picture*. The *evolution in the interaction picture* is

$$U_{\rm Int}(t_+,t_-) \;:=\; {\rm e}^{{\rm i}t_+H_{\rm fr}}U(t_+,t_-){\rm e}^{-{\rm i}t_-H_{\rm fr}}.$$

Note that $U_{\rm Int}(t,t)=\mathbb{1}$ and

$$\frac{\rm d}{{\rm d}t_+}U_{\rm Int}(t_+,t_-) = -{\rm i}H_{\rm Int}(t_+)U_{\rm Int}(t_+,t_-); \tag{11.30}$$

$$\frac{\rm d}{{\rm d}t_-}U_{\rm Int}(t_+,t_-) = U_{\rm Int}(t_+,t_-){\rm i}H_{\rm Int}(t_-), \tag{11.31}$$

where the Hamiltonian for the interaction picture is

$$H_{\rm Int}(t) = {\rm e}^{{\rm i}tH_{\rm fr}}V(t){\rm e}^{-{\rm i}tH_{\rm fr}}. \tag{11.32}$$

Therefore, we can write

$$U_{\rm Int}(t_+,t_-) \;=\; {\rm Texp}\left(-{\rm i}\int_{t_-}^{t_+}H_{\rm Int}(t){\rm d}t\right).$$

Thus if

$$\begin{aligned}\rho_{\rm Int}(t) &= U_{\rm Int}(t,0)\rho U_{\rm Int}(0,t)\\ &= {\rm e}^{{\rm i}tH_{\rm fr}}U(t,0)\rho U(0,t){\rm e}^{-{\rm i}tH_{\rm fr}}, \qquad (11.33)\\ A_{\rm fr}(t) &= {\rm e}^{{\rm i}tH_{\rm fr}}A{\rm e}^{-{\rm i}tH_{\rm fr}}, \qquad (11.34)\end{aligned}$$

then the expectation value (11.13) coincides with

$${\rm Tr}A_{\rm fr}(t)\rho_{\rm Int}(t). \tag{11.35}$$

We define the *scattering operator* by

$$\begin{aligned}S \;&:=\; \lim_{t_+,-t_-\to\infty}U_{\rm Int}(t_+,t_-)\\ &=\; {\rm Texp}\left(-{\rm i}\int_{-\infty}^{\infty}H_{\rm Int}(t){\rm d}t\right). \qquad (11.36)\end{aligned}$$

We also introduce the *Møller operators*

$$\begin{aligned}S^- \;&:=\; \lim_{t\to\infty}U(0,-t){\rm e}^{{\rm i}tH_{\rm fr}} = \lim_{t\to\infty}U_{\rm Int}(0,-t)\\ &=\; {\rm Texp}\left(-{\rm i}\int_{-\infty}^{0}H_{\rm Int}(t){\rm d}t\right), \qquad (11.37)\\ S^+ \;&:=\; \lim_{t\to\infty}U(0,t){\rm e}^{-{\rm i}tH_{\rm fr}} = \lim_{t\to\infty}U_{\rm Int}(0,t)\\ &=\; {\rm Texp}\left(-{\rm i}\int_{0}^{\infty}H_{\rm Int}(t){\rm d}t\right)^{-1}. \qquad (11.38)\end{aligned}$$

Clearly, $S = S^{+(-1)}S^{-}$.

Note that both Møller operators and the scattering operator trivially exist if $V(t)$ decays sufficiently fast as $|t| \to \infty$. In fact, this is a typical situation in QFT, where we usually impose a temporal "adiabatic cutoff".

In quantum mechanics one often applies this formalism to time independent potentials, but this is a different story.

The interaction picture described above has also its "Heisenberg picture version":

$$U^{\mathrm{Hp}}_{\mathrm{Int}}(t_+, t_-) := U(0, t_+)\mathrm{e}^{-\mathrm{i}(t_+ - t_-)H_{\mathrm{fr}}}U(t_-, 0) \tag{11.39}$$

$$= \mathrm{Texp}\left(- \int_{t_-}^{t_+} H^{\mathrm{Hp}}_{\mathrm{Int}}(t)\mathrm{d}t \right), \tag{11.40}$$

$$H^{\mathrm{Hp}}_{\mathrm{Int}}(t) := U_{\mathrm{Int}}(0, t)H_{\mathrm{Int}}(t)U_{\mathrm{Int}}(t, 0) = U(0, t)V(t)U(t, 0). \tag{11.41}$$

12 Euclidean fields and spectral shift function

12.1 Trace

Let A be a positive operator on a Hilbert space $\mathcal{H}$. Let $\{e_i,\ i \in I\}$ be an orthonormal basis in $\mathcal{H}$. One can show that

$$\mathrm{Tr}A := \sum_{i \in I} (e_i | Ae_i) \tag{12.1}$$

does not depend on the choice of a basis and defines a number $\in [0, \infty]$ called the *trace* of A. We say that A is *trace class* if $\mathrm{Tr}A < \infty$.

If A is any operator, then it is *trace class* if it can be written as a linear combination of positive trace class operators

$$A_i = \sum_{i=1}^{n} c_i A_i. \tag{12.2}$$

Then one sets

$$\mathrm{Tr}A = \sum_{i=1}^{n} c_i \mathrm{Tr}A_i. \tag{12.3}$$

One can show that (12.3) does not depend on the decomposition (12.2). Note that for any unitary U

$$\mathrm{Tr}A = \mathrm{Tr}UAU^*. \tag{12.4}$$

If A is an operator on $L^2(\mathbb{R}^d)$, and $A(x, y)$ is its distributional kernel, then under some conditions one can show that

$$\mathrm{Tr}A = \int A(x, x)\mathrm{d}x. \tag{12.5}$$

For instance, if $A = f(\hat{x})g(\hat{p})$, then

$$A(x,y) = \int f(x)g(p)\mathrm{e}^{\mathrm{i}(x-y)p}\frac{\mathrm{d}p}{(2\pi)^d}, \qquad \mathrm{Tr}A = \int f(x)g(p)\frac{\mathrm{d}x\mathrm{d}p}{(2\pi)^d}. \tag{12.6}$$

Suppose that A is an operator such that $]-\infty, 0]$ is disjoint from its spectrum. Then we can define $\ln(A)$. Suppose in addition that $A - \mathbb{1}$ is trace class. Then it is easy to show that $\ln(A)$ is trace class. We then can define the so-called *Fredholm determinant of A*:

$$\det A := \mathrm{e}^{\mathrm{Tr}\ln(A)}. \tag{12.7}$$

12.2 Neutral Euclidean fields

Suppose that $I(\phi)$ is a function of (classical) fields describing the Hamiltonian (or the "Euclidean Action for a field theory"). Then

$$\int \mathrm{e}^{-\beta I(\phi)}\mathrm{D}\phi \tag{12.8}$$

is called the *partition function*. The parameter β has the interpretation of $\frac{1}{kT}$, where T is the temperature. Anyway, we will assume $\beta = 1$.

In many situations, e.g. the thermodynamic limit, the partition function is infinite and instead it is more natural to consider the ratio of partition functions for two Hamiltonians, I and I_0. We can then introduce the parameter $\mathcal{E}$ equal to the logarithm of its relative partition function:

$$\mathrm{e}^{-\mathcal{E}} := \frac{\int \mathrm{e}^{-I(\phi)}\mathrm{D}\phi}{\int \mathrm{e}^{-I_0(\phi)}\mathrm{D}\phi}. \tag{12.9}$$

Depending on circumstances, $\mathcal{E}$ is called the free energy, pressure or effective action.

Consider $\mathbb{R}^4$ with the Euclidean signature and the Euclidean neutral field with the mass squared perturbed by $\kappa \in \mathcal{S}(\mathbb{R}^4)$:

$$I(\phi) = \int \frac{1}{2}\big(\partial_\mu\phi(x)\partial^\mu\phi(x) + m^2\phi^2(x) + \kappa(x)\phi^2(x)\big)\mathrm{d}x \tag{12.10}$$

$$I_0(\phi) = \int \frac{1}{2}\big(\partial_\mu\phi(x)\partial^\mu\phi(x) + m^2\phi^2(x)\big)\mathrm{d}x. \tag{12.11}$$

We would like to compute the renormalized value of $\mathcal{E}$. Formally we have

$$\mathrm{e}^{-\mathcal{E}} = \Big(\frac{\det(\hat{p}^2+m^2)}{\det(\hat{p}^2+m^2+\kappa(\hat{x}))}\Big)^{\frac{1}{2}} = \det\Big(\mathbb{1} + \kappa(\hat{x})(\hat{p}^2+m^2)^{-1}\Big)^{-\frac{1}{2}}, \tag{12.12}$$

$$\begin{aligned}\mathcal{E} =& \frac{1}{2}\mathrm{Tr}\big(\log(\hat{p}^2+m^2+\kappa(\hat{x})) - \log(\hat{p}^2+m^2)\big)\\ =& \frac{1}{2}\mathrm{Tr}\log\big(\mathbb{1} + \kappa(\hat{x})(\hat{p}^2+m^2)^{-1}\big).\end{aligned} \tag{12.13}$$

Unfortunately, (12.13) are divergent. We will show how to renormalize $\mathcal{E}$. This means, we will show how to modify the Hamiltonian by adding local counterterms so that we obtain a finite expression.

Let us try to analyze $\mathcal{E}$, in spite of the fact that it is ill defined. We have

$$\mathcal{E} \quad = \quad \sum_{n=1}^{\infty} \frac{(-1)^{n+1}}{2n} \mathrm{Tr}\big(\kappa(\hat{x})(\hat{p}^2+m^2)^{-1}\big)^n =: \sum_{n=1}^{\infty} \mathcal{E}_n.$$

Let us compare this with the classical approximation of $\mathcal{E}$:

$$\mathcal{E}^{\mathrm{cl}} := \frac{1}{2}\int \big(\log(p^2+m^2+\kappa(x)\big) - \log(p^2+m^2)\big)\frac{\mathrm{d}x\mathrm{d}p}{(2\pi)^4} \tag{12.14}$$

$$= \sum_{n=1}^{\infty} \frac{(-1)^{n+1}}{2n} \int \big(\kappa(x)(p^2+m^2)^{-1}\big)^n \frac{\mathrm{d}x\mathrm{d}p}{(2\pi)^4} =: \sum_{n=1}^{\infty} \mathcal{E}_n^{\mathrm{cl}}. \tag{12.15}$$

Note that

$$\mathcal{E}_1 = \mathcal{E}_1^{\mathrm{cl}} = \frac{1}{2}\int \kappa(x)\mathrm{d}x \int \frac{\mathrm{d}p}{(2\pi)^4(p^2+m^2)} \tag{12.16}$$

is divergent. But the classical and quantum quantities coincide. We will simply drop them.

$\mathcal{E}_2$ and $\mathcal{E}_2^{\mathrm{cl}}$ are also divergent, but in general different:

$$-\mathcal{E}_2 = \frac{1}{4}\mathrm{Tr}\Big(\kappa(\hat{x})(\hat{p}^2+m^2)^{-1}\kappa(\hat{x})(\hat{p}^2+m^2)^{-1}\Big)$$

$$= \frac{1}{4}\int \kappa(p_1-p_2)\frac{\mathrm{d}p_2}{(2\pi)^4(p_2^2+m^2)}\kappa(p_2-p_1)\frac{\mathrm{d}p_1}{(2\pi)^4(p_1^2+m^2)} \tag{12.17}$$

$$= \frac{1}{4}\int \frac{\mathrm{d}k}{(2\pi)^4}\frac{\mathrm{d}q}{(2\pi)^4}\frac{|\kappa(k)|^2}{((q+\frac{1}{2}k)^2+m^2)((q-\frac{1}{2}k)^2+m^2)} \tag{12.18}$$

$$= \int |\kappa(k)|^2 \pi(k^2)\frac{\mathrm{d}k}{(2\pi)^4}, \tag{12.19}$$

$$-\mathcal{E}_2^{\mathrm{cl}} = \frac{1}{4}\int\int \kappa(x)^2\mathrm{d}x\frac{\mathrm{d}p}{(2\pi)^4(p^2+m^2)^2} \tag{12.20}$$

$$= \frac{1}{4}\int\int |\kappa(k)|^2 \frac{\mathrm{d}k}{(2\pi)^4}\frac{\mathrm{d}p}{(2\pi)^4(p^2+m^2)^2}, \tag{12.21}$$

$$= \int |\kappa(k)|^2\pi(0)\frac{\mathrm{d}k}{(2\pi)^4}, \tag{12.22}$$

where in (12.18) and (12.19) we used $\kappa(-k) = \overline{\kappa(k)}$ and we set $p_1 = q - \frac{1}{2}k$, $p_2 = q + \frac{1}{2}k$, and we introduced

$$\pi(k^2) = \frac{1}{4}\int \frac{\mathrm{d}^4q}{(2\pi)^4}\frac{1}{((q+\frac{1}{2}k)^2+m^2)((q-\frac{1}{2}k)^2+m^2)}, \tag{12.23}$$

We will see that the following renormalized expressions are finite:

$$\mathcal{E}_2^{\mathrm{ren}} := \mathcal{E}_2 - \mathcal{E}_2^{\mathrm{cl}} = \int |\kappa(k)|^2 \pi^{\mathrm{ren}}(k^2)\frac{\mathrm{d}k}{(2\pi)^4}, \tag{12.24}$$

$$\pi^{\mathrm{ren}}(k^2) := \pi(k^2) - \pi(0). \tag{12.25}$$

All the terms $\mathcal{E}_n$ and $\mathcal{E}_n^{\rm cl}$ with $n \geq 3$ are convergent.

To rigorously define the above expressions we need first to perform some kind of regularization. For instance, we can use the the *Pauli-Villars method* with $m_0 = m$, $C_0 = 1$, $m_1 = M$, and $C_1 = -1$. (See Subsection 12.4 for more about this method). Let us set $\pi(m, k^2)$ to be the formal expression (12.23). Set

$$\pi^{\rm reg}(k^2) := \pi(m, k^2) - \pi(M, k^2) = \sum_{i=0}^{1} C_i \pi(m_i, k^2). \tag{12.26}$$

(12.26) is given by a convergent integrals. The rigorous definition of $\pi^{\rm ren}(k^2)$ is

$$\pi^{\rm ren}(k^2) := \lim_{M\to\infty} \big(\pi^{\rm reg}(k^2) - \pi^{\rm reg}(0)\big). \tag{12.27}$$

We will compute $\pi^{\rm ren}(k^2)$.

In order not to clutter the formulas, in the following computations we use the ill defined $\pi(k^2)$. The following formulas become well defined when we replace m with m_i and insert $\sum_{i=0}^{1} C_i$, so that instead of $\pi(k^2)$ we obtain $\pi^{\rm reg}(k^2)$:

$$\begin{aligned}
4\pi(k^2) \;&=\; \int \frac{\mathrm{d}^4 q}{(2\pi)^4} \frac{1}{((q+\frac{1}{2}k)^2+m^2)((q-\frac{1}{2}k)^2+m^2)} \\
&= \int \frac{\mathrm{d}^4 q}{(2\pi)^4} \int_0^\infty \mathrm{d}\alpha_1 \int_0^\infty \mathrm{d}\alpha_2 \exp\left(-(\alpha_1+\alpha_2)\Big(q^2+\frac{1}{4}k^2+m^2\Big) - (\alpha_1-\alpha_2)qk\right) \\
&= \frac{1}{(4\pi)^2} \int_0^\infty \mathrm{d}\alpha_1 \int_0^\infty \mathrm{d}\alpha_2 \frac{1}{(\alpha_1+\alpha_2)^2} \exp\left(-(\alpha_1+\alpha_2)m^2 - \frac{\alpha_1\alpha_2}{\alpha_1+\alpha_2}k^2\right) \\
&= \frac{1}{(4\pi)^2 2} \int_{-1}^1 \mathrm{d}v \int_0^\infty \frac{\mathrm{d}\rho}{\rho} \exp\left(-\rho\left(m^2 + \frac{(1-v^2)k^2}{4}\right)\right) \\
&= \frac{1}{(4\pi)^2 2} \int_{-1}^1 \mathrm{d}v \log\left(m^2 + \frac{k^2(1-v^2)}{4}\right) \\
&= \frac{1}{(4\pi)^2 2} \int_{-1}^1 \mathrm{d}v \left(\log\left(1 + \frac{(1-v^2)k^2}{4m^2}\right) + \log m^2\right).
\end{aligned}$$

We used the identities (12.28) and (12.29):

$$\frac{1}{A} \;=\; \int_0^\infty \mathrm{d}\alpha \exp(-\alpha A), \tag{12.28}$$

$$\int \frac{\mathrm{d}p}{(2\pi)^4} \exp\big(-(ap^2+bp)\big) \;=\; \frac{1}{(4\pi)^2 a^2} \exp\big(b^2/4a\big). \tag{12.29}$$

Then we changed the variables to

$$\alpha_1 = \rho\frac{(1-v)}{2}, \quad \alpha_2 = \rho\frac{(1+v)}{2}, \tag{12.30}$$

$$\text{so that} \quad \alpha_1+\alpha_2 = \rho, \quad -\alpha_1+\alpha_2 = \rho v, \qquad \mathrm{d}\alpha_1 \mathrm{d}\alpha_2 = \frac{1}{2}\rho \mathrm{d}v \mathrm{d}\rho.$$

At the end we use the identity (12.31):

$$\int_0^\infty \sum_i C_i \frac{\mathrm{d}\rho}{\rho} \mathrm{e}^{-\rho A_i} = -\sum_i C_i \log(A_i). \tag{12.31}$$

valid if $\sum C_i = 0$.

Now the *renormalized* π is given by

$$\begin{aligned}
\pi^{\mathrm{ren}}(k^2) &:= \lim_{M\to\infty} \big(\pi^{\mathrm{reg}}(k^2) - \pi^{\mathrm{reg}}(0)\big) \\
&= \lim_{M\to\infty} \frac{1}{4(4\pi)^2 2} \int_{-1}^{1} \Big(\log\Big(1 + \frac{k^2(1-v^2)}{4m^2}\Big) - \log\Big(1 + \frac{k^2(1-v^2)}{4M^2}\Big)\Big)\mathrm{d}v \\
&= \frac{1}{4(4\pi)^2 2} \int_{-1}^{1} \log\Big(1 + \frac{k^2(1-v^2)}{4m^2}\Big)\mathrm{d}v.
\end{aligned} \tag{12.32}$$

Note that

$$\pi^{\mathrm{ren}}(0) = 0, \tag{12.33}$$

which is our *renormalization condition*. Finally, we evaluate π^{ren} using

$$\int \log(1-w^2)\mathrm{d}w = w\log(1-w^2) - 2w + \log\frac{(1+w)}{(1-w)}, \quad 0 < w < 1. \tag{12.34}$$

We obtain

$$\pi^{\mathrm{ren}}(k^2) = \frac{1}{4(4\pi)^2}\Big(\frac{1}{\theta}\log\frac{1+\theta}{1-\theta} - 2\Big), \qquad \theta = \sqrt{\frac{k^2}{k^2+4m^2}}. \tag{12.35}$$

Here are operator-theoretic formulas for the renormalized quantities:

$$\begin{aligned}
\mathcal{E}_2^{\mathrm{ren}} &= -\frac{1}{4}\mathrm{Tr}\Big(\big(\kappa(x)(\hat{p}^2+m^2)^{-1}\big)^2 - \kappa(x)^2(\hat{p}^2+m^2)^{-2}\Big), \\
\mathcal{E}^{\mathrm{ren}} &= \frac{1}{2}\mathrm{Tr}\Big(\log\big(\mathbb{1} + \kappa(x)(\hat{p}^2+m^2)^{-1}\big) - \kappa(x)(\hat{p}^2+m^2)^{-1} \\
&\qquad + \frac{1}{2}\kappa^2(x)(\hat{p}^2+m^2)^{-2}\Big).
\end{aligned} \tag{12.36}$$

12.3 Charged Euclidean fields

Consider Euclidean charged field on $\mathbb{R}^4$ in the presence of magnetic potential $[A_\mu]$. Formally we have

$$\begin{aligned}
&\frac{\int \exp\Big(-\int\Big(\big(\partial_\mu + \mathrm{i}eA_\mu(x)\big)\psi(x)\Big)^*\big(\partial^\mu + \mathrm{i}eA^\mu(x)\big)\psi(x) + m^2\psi^*(x)\psi(x)\Big)\mathrm{d}x\Big)\mathrm{D}\psi^*\mathrm{D}\psi}{\int \exp\Big(-\int\big(\partial_\mu\psi^*(x)\partial^\mu\psi(x) + m^2\psi^*(x)\psi(x)\big)\mathrm{d}x\Big)\mathrm{D}\psi^*\mathrm{D}\psi} \\
=&\frac{\det K_0}{\det K} = \exp\Big(-\mathrm{Tr}\big(\log(K) - \log(K_0)\big)\Big),
\end{aligned} \tag{12.37}$$

where

$$K_0 := \hat{p}^2 + m^2, \qquad K := -\big(\partial^\mu + \mathrm{i}eA^\mu(x)\big)\big(\partial_\mu + \mathrm{i}eA_\mu(x)\big) + m^2. \tag{12.38}$$

are operators on $L^2(\mathbb{R}^4)$.

Our goal is to compute the renormalized value of

$$\mathcal{E} := \mathrm{Tr}\big(\log(K) - \log(K_0)\big). \tag{12.39}$$

We have

$$\begin{aligned}\mathcal{E} =& \mathrm{Tr}\log\Big(\mathbb{1} + \big(-\mathrm{i}eA^\mu\partial_\mu - \mathrm{i}e\partial_\mu A^\mu + e^2A_\mu A^\mu\big)(\hat{p}^2+m^2)^{-1}\Big) \qquad (12.40)\\ =& \sum_{n=1}^{\infty}\frac{(-1)^{n+1}}{n}\mathrm{Tr}\Big(\big(-\mathrm{i}eA^\mu\partial_\mu - \mathrm{i}e\partial_\mu A^\mu + e^2A_\mu A^\mu\big)(\hat{p}^2+m^2)^{-1}\Big)^n.\end{aligned}$$

We have $\overline{\mathcal{E}(A)} = \mathcal{E}(-A)$. Besides, $\mathcal{E}(A)$ is real (because of the self-adjointness of K and K_0). Therefore, terms of odd order in e vanish. This is the content of *Furry's theorem* for charged bosons. Hence (12.40) can be written as

$$\mathcal{E} = \sum_{n=1}^{\infty} e^{2n}\mathcal{E}_n.$$

The expressions for $\mathcal{E}_n$ are convergent for $n \geq 3$. $\mathcal{E}_2$ is logarithmically divergent, but its physically relevant gauge invariant part is convergent. $\mathcal{E}_1$ is quadratically divergent and its gauge-invariant part is logarithmically divergent. It needs an infinite renormalization, which will be described below.

The lowest nonzero terms are of the second order in e, and hence of the first order in $\alpha = \frac{e^2}{4\pi}$.

$$\begin{aligned}-2e^2\mathcal{E}_1 = e^2\int (p_1+p_2)^\mu A_\mu(p_1-p_2)\frac{\mathrm{d}p_2}{(2\pi)^4(p_2^2+m^2)}&\\ \times (p_2+p_1)^\nu A_\nu(p_2-p_1)\frac{\mathrm{d}p_1}{(2\pi)^4(p_1^2+m^2)} \qquad (12.41)&\\ - e^2\int 2A_\mu(-k)A^\mu(k)\frac{\mathrm{d}k}{(2\pi)^4}\frac{\mathrm{d}p}{(2\pi)^4(p^2+m^2)} \qquad (12.42)&\\ =: \int \frac{\mathrm{d}k}{(2\pi)^4}A^\mu(-k)A^\nu(k)2\Pi_{\mu\nu}(k). \qquad (12.43)&\end{aligned}$$

(12.43) defines the *vacuum energy tensor* $\Pi_{\mu\nu}(k)$.

We will compute $\Pi_{\mu\nu}(k)$ using the *Pauli-Villars regularization*. The ultraviolet problem is more severe now than it was for the mass-like perturbation, where a single additional fictitious particle sufficed to make the expressions well defined. Now we need two fictitious particles:

$$\begin{aligned} m_0^2 &:= m^2, & C_0 &:= 1,\\ m_1^2 &:= m^2 + 2\Lambda^2, & C_1 &:= 1,\\ m_2^2 &:= m^2 + \Lambda^2, & C_2 &:= -2.\end{aligned}$$

Using

$$\sum_{i=0}^{2} C_i = \sum_{i=0}^{2} C_i m_i^2 = 0 \tag{12.44}$$

we can check that with this choice the sums used in the following computations are integrable.

$$\begin{aligned}
2\Pi_{\mu\nu}(k) &= e^2 \int \frac{\mathrm{d}^4 q}{(2\pi)^4} \Big(\frac{4 q_\mu q_\nu}{\big((q+\frac{1}{2}k)^2 + m_i^2 - \mathrm{i}0\big)\big((q-\frac{1}{2}k)^2 + m^2\big)} \\
&\qquad - \frac{g_{\mu\nu}}{\big((q+\frac{1}{2}k)^2 + m^2\big)} - \frac{g_{\mu\nu}}{\big((q-\frac{1}{2}k)^2 + m^2\big)} \Big) \\
&= e^2 \int \frac{\mathrm{d}^4 q}{(2\pi)^4} \frac{4 q_\mu q_\nu - 2 g_{\mu\nu}(q^2 + \frac{1}{4}k^2 + m^2)}{\big((q+\frac{1}{2}k)^2 + m^2\big)\big((q-\frac{1}{2}k)^2 + m^2\big)} \\
&= e^2 \int \frac{\mathrm{d}^4 q}{(2\pi)^4} \int_0^\infty \mathrm{d}\alpha_1 \int_0^\infty \mathrm{d}\alpha_2 \left(4 q_\mu q_\nu - 2 g_{\mu\nu} \Big(q^2 + \frac{1}{4}k^2 + m^2 \Big) \right) \\
&\qquad \times \exp\left(-(\alpha_1 + \alpha_2) \Big(q^2 + \frac{1}{4}k^2 + m^2 \Big) - (\alpha_1 - \alpha_2) q k \right) \\
&= e^2 \int \frac{\mathrm{d}^4 q}{(2\pi)^4} \int_0^\infty \mathrm{d}\alpha_1 \int_0^\infty \mathrm{d}\alpha_2 \left(4 \partial_{z_\mu} \partial_{z_\nu} - 2 g_{\mu\nu} \Big(\partial_z^2 + \frac{1}{4}k^2 + m^2 \Big) \right) \\
&\qquad \times \exp\left(-(\alpha_1 + \alpha_2) \Big(q^2 + \frac{1}{4}k^2 + m^2 \Big) - (\alpha_1 - \alpha_2) q k + z q \right) \Big|_{z=0} \\
&= \frac{e^2}{(4\pi)^2} \int_0^\infty \mathrm{d}\alpha_1 \int_0^\infty \mathrm{d}\alpha_2 \frac{1}{(\alpha_1 + \alpha_2)^2} \left(4 \partial_{z_\mu} \partial_{z_\nu} - 2 g_{\mu\nu} \Big(\partial_z^2 + \frac{1}{4}k^2 + m^2 \Big) \right) \\
&\qquad \times \exp\left(-(\alpha_1 + \alpha_2) \Big(\frac{1}{4}k^2 + m^2 \Big) + \frac{1}{4(\alpha_1 + \alpha_2)} \Big((\alpha_1 - \alpha_2) k - z \Big)^2 \right) \Big|_{z=0}
\end{aligned}$$

$$\begin{aligned}
&= \frac{e^2}{(4\pi)^2} \int_0^\infty \mathrm{d}\alpha_1 \int_0^\infty \mathrm{d}\alpha_2 \Bigg(- \frac{(\alpha_1 - \alpha_2)^2}{(\alpha_1 + \alpha_2)^4} (g_{\mu\nu} k^2 - k_\mu k_\nu) \\
&\qquad - 2 g_{\mu\nu} \left(\frac{\alpha_1 \alpha_2}{(\alpha_1 + \alpha_2)^4} k^2 + \frac{1}{(\alpha_1 + \alpha_2)^3} + \frac{m^2}{(\alpha_1 + \alpha_2)^2} \right) \Bigg) \\
&\qquad \times \exp\left(-(\alpha_1 + \alpha_2) m^2 - \frac{\alpha_1 \alpha_2}{\alpha_1 + \alpha_2} k^2 \right) \\
&=: (-g_{\mu\nu} k^2 + k_\mu k_\nu) 2\Pi^{\mathrm{gi}}(k^2) + 2\Pi^{\mathrm{gd}}_{\mu\nu}(k^2).
\end{aligned}$$

Let us compute the gauge dependent part of the vacuum energy tensor:

$$
\begin{aligned}
&\Pi^{\rm gd}_{\mu\nu}(k^2)\\
=&\frac{e^2}{(4\pi)^2}\int_0^\infty {\rm d}\alpha_1\int_0^\infty {\rm d}\alpha_2\exp\left(-(\alpha_1+\alpha_2)m^2-\frac{\alpha_1\alpha_2}{\alpha_1+\alpha_2}k^2\right)\\
&\times g_{\mu\nu}\left(\frac{\alpha_1\alpha_2k^2}{(\alpha_1+\alpha_2)^4}+\frac{1}{(\alpha_1+\alpha_2)^3}+\frac{m^2}{(\alpha_1+\alpha_2)^2}\right)\\
=&\frac{e^2}{(4\pi)^22}\int_{-1}^1{\rm d}v\int_0^\infty{\rm d}\rho\exp\left(-\rho m^2-\frac{(1-v^2)\rho}{4}k^2\right)g_{\mu\nu}\left(\frac{(1-v^2)}{4\rho}k^2+\frac{1}{\rho^2}+\frac{m^2}{\rho}\right)\\
=&-\frac{e^2}{(4\pi)^22}\int_{-1}^1{\rm d}v\int_0^\infty{\rm d}\rho\frac{\rm d}{{\rm d}\rho}\frac{1}{\rho}\exp\left(-\rho m^2-\frac{(1-v^2)\rho}{4}k^2\right)g_{\mu\nu}\\
=&-\frac{e^2}{(4\pi)^22}\int_{-1}^1{\rm d}v\frac{1}{\rho}\exp\left(-\rho m^2-\frac{(1-v^2)\rho}{4}k^2\right)g_{\mu\nu}\Big|_{\rho=0}^{\rho=\infty}.
\end{aligned}
$$

It vanishes (remember to insert the sum including "fictitious particles"!). To compute the gauge invariant part we proceed similarly as in Subsection 12.2, and we obtain

$$
\begin{aligned}
\Pi^{\rm gi}(k^2) &= \frac{e^2}{2(4\pi)^2}\int_0^\infty{\rm d}\alpha_1\int_0^\infty{\rm d}\alpha_2\frac{(\alpha_1-\alpha_2)^2}{(\alpha_1+\alpha_2)^4}\\
&\quad\times\exp\left(-(\alpha_1+\alpha_2)m^2-\frac{\alpha_1\alpha_2}{\alpha_1+\alpha_2}k^2\right)\\
&= \frac{e^2}{4(4\pi)^2}\int_{-1}^1{\rm d}v\int_0^\infty\frac{{\rm d}\rho}{\rho}v^2\exp\left(-\rho\left(m^2+\frac{(1-v^2)k^2}{4}\right)\right)\\
&= \frac{e^2}{4(4\pi)^2}\int_{-1}^1{\rm d}vv^2\log\left(m^2+\frac{(1-v^2)k^2}{4}\right).
\end{aligned}
$$

We define

$$
\begin{aligned}
\Pi^{\rm ren}(k^2) &:= \lim_{\Lambda\to\infty}\left(\Pi^{\rm gi}(k^2)-\Pi^{\rm gi}(0)\right) \qquad (12.45)\\
&= \frac{e^2}{4(4\pi)^2}\int_{-1}^1{\rm d}vv^2\log\left(1+\frac{(1-v^2)k^2}{4m^2}\right).
\end{aligned}
$$

Using

$$
\begin{aligned}
\int w^2\log(1-w^2){\rm d}w =&\frac{w^3}{3}\log(1-w^2)-\frac{2w^3}{9}-\frac{2w}{3}\\
&+\frac{1}{3}\log\frac{(1+w)}{(1-w)},\quad 0<w<1, \qquad (12.46)
\end{aligned}
$$

we obtain

$$
\begin{aligned}
&\Pi^{\rm ren}(k^2)\\
=&\frac{e^2}{2\cdot3(4\pi)^2}\left(\frac{1}{\theta^3}\log\frac{1+\theta}{1-\theta}-\frac{2}{3}-\frac{2}{\theta^2}\right),\qquad \theta=\sqrt{\frac{k^2}{k^2+4m^2}}.
\end{aligned}
$$

Note that the Fourier transform of the electromagnetic field is

$$F_{\mu\nu}(k) = k_\mu A_\nu(k) - k_\nu A_\mu(k). \tag{12.47}$$

Hence

$$-\frac{1}{2}\overline{F_{\mu\nu}(k)}F^{\mu\nu}(k) = -k^2|A(k)|^2 + |kA(k)|^2. \tag{12.48}$$

Thus the renormalized 1st order contribution to the vacuum energy is

$$\mathcal{E}_1^{\rm ren} = -\int \frac{\mathrm{d}k}{2(2\pi)^4}\Pi^{\rm ren}(k^2)\overline{F_{\mu\nu}(k)}F^{\mu\nu}(k). \tag{12.49}$$

with the renormalization condition

$$\Pi^{\rm ren}(0) = 0. \tag{12.50}$$

12.4 Spectral shift function

Suppose H and H_0 be two self-adjoint operators. We say that the pair H, H_0 *possesses the spectral shift function* if for any $f \in C_{\rm c}^\infty(\mathbb{R})$, the operator $f(H) - f(H_0)$ is trace class. Clearly, the map

$$C_{\rm c}^\infty(\mathbb{R}) \ni f \mapsto f(H) - f(H_0) \in \mathbb{R} \tag{12.51}$$

is a linear functional. Under some conditions on H, H_0 there exists a function $\xi(s) = \xi_{H,H_0}(s)$ such that

$$\mathrm{Tr}\big(f(H) - f(H_0)\big) = \int \xi(s) f'(s)\mathrm{d}s. \tag{12.52}$$

$\xi(s)$ is defined up to an additive constant. If H, H_0 are bounded from below, which will always be true in our applications, then one can assume that $\lim\limits_{s\to-\infty}\xi(s) = 0$. $\xi_{H,H_0}(s)$ is called the *spectral shift function*.

Suppose for the moment that H, H_0 are trace class. Then they can be diagonalized. Let E_n, $E_{0,n}$ be the eigenvalues of H, resp. H_0, in the increasing order, counting with multiplicities. Then

$$\mathrm{Tr}\big(f(H) - f(H_0)\big) = \sum_{n=1}^\infty \big(f(E_n) - f(E_{0,n})\big) = \sum_{n=1}^\infty \int_{E_{0,n}}^{E_n} f'(s)\mathrm{d}s, \tag{12.53}$$

which explains the name "spectral shift function".

Let us describe the basic method of computing the spectral shift. Let us write $H = H_0 + \lambda V$. We introduce

$$\begin{aligned} D_{H,H_0}(z) = D(z) :&= \mathrm{Tr}\big(\log(H-z) - \log(H_0 - z)\big) \\ &= \mathrm{Tr}\log\big((H-z)(H_0-z)^{-1}\big) = \mathrm{Tr}\log(\mathbb{1} + \lambda V(H_0-z)^{-1}\big) \\ &= \sum_{n=1}^\infty \frac{\lambda^n(-1)^{n+1}}{n}\mathrm{Tr}\big(V(H_0-z)\big)^n. \end{aligned}$$

Clearly, if the spectral shift function is well defined, then

$$D(z) = \int \xi(s)(s-z)^{-1}\mathrm{d}s, \tag{12.54}$$

which can be inverted:

$$\xi(s) = \frac{1}{2\pi\mathrm{i}}\big(D(s+\mathrm{i}0) - D(s-\mathrm{i}0)\big). \tag{12.55}$$

This method can fail if the rhs of (12.54) is not integrable. Suppose that $n \in \mathbb{N}$, the spectral shift exists and satisfies

$$\int |\xi(s)|(|s|+1)^{-n-1}\mathrm{d}s < \infty. \tag{12.56}$$

Then there exists an improved method of computing the spectral shift, which is essentially an adaptation of the Pauli-Villars method from QFT. Choose $c_0, , \dots c_n$ and $\Lambda_0, \dots, \Lambda_n$ such that

$$\begin{aligned} c_0 + \cdots + c_n &= 0, \\ c_0\Lambda_0 + \cdots + c_n\Lambda_n &= 0, \\ &\cdots \\ c_0\Lambda_0^n + \cdots + c_n\Lambda_n^n &= 0. \end{aligned}$$

Now we easily check that for $s \to \infty$

$$\sum_{i=0}^{n} c_i(s+\Lambda_i - z)^{-1} = O(s^{-1-n}), \tag{12.57}$$

Hence

$$\begin{aligned} D^{\mathrm{reg}}(z) :=& \mathrm{Tr}\Big(\log \prod_{i=0}^{n}(H+\Lambda_i - z)^{c_i} - \log \prod_{i=0}^{n}(H_0+\Lambda_i - z)^{c_i}\Big) \\ &= \int \xi(s) \sum_{i=0}^{n} c_i(s+\Lambda_i - z)^{-1}\mathrm{d}s. \end{aligned} \tag{12.58}$$

is well defined. Now

$$\sum_{i=0}^{n} c_i\xi(s+\Lambda_i) = \frac{1}{2\pi\mathrm{i}}\big(D^{\mathrm{reg}}(s+\mathrm{i}0) - D^{\mathrm{reg}}(s-\mathrm{i}0)\big). \tag{12.59}$$

In practice, we set $c_0 = 1$, $\Lambda_0 = 0$, $\Lambda_i = \alpha_i\Lambda$ with c_i and $\alpha_i > 0$ fixed for $i = 1, \dots, n$. Then

$$\xi(s) = \lim_{\Lambda\to\infty} \frac{1}{2\pi\mathrm{i}}\big(D^{\mathrm{reg}}(s+\mathrm{i}0) - D^{\mathrm{reg}}(s-\mathrm{i}0)\big). \tag{12.60}$$

13 Scalar field with a masslike perturbation

13.1 Lagrangian and Hamiltonian formalism

Consider the Lagrangian density

$$\mathcal{L}(x) = -\frac{1}{2}\partial_\mu\phi(x)\partial^\mu\phi(x) - \frac{1}{2}(m^2 + \kappa(x))\phi(x)^2, \tag{13.1}$$

where $\mathbb{R}^{1,3} \ni x \mapsto \kappa(x)$ is a given function. In most of this subsection we will assume that κ is Schwartz and $m > 0$. (13.1) leads to the equations

$$(-\Box + m^2)\phi(x) = -\kappa(x)\phi(x), \tag{13.2}$$

The variable conjugate to $\phi(x)$ is $\pi(x) := \dot{\phi}(x)$, so that

$$\begin{aligned} \{\phi(t,\vec{x}),\phi(t,\vec{y})\} = \{\pi(t,\vec{x}),\pi(t,\vec{y})\} &= 0, \\ \{\phi(t,\vec{x}),\pi(t,\vec{y})\} &= \delta(\vec{x}-\vec{y}). \end{aligned} \tag{13.3}$$

The theory of the Klein-Gordon equation with a variable mass is very similar to the one with a constant mass. We can define the corresponding retarded and advanced propagators as the unique distributional solutions of

$$\big(-\Box_x + m^2 + \kappa(x)\big)G^{\vee/\wedge}(x,y) = \delta(x-y), \tag{13.4}$$

satisfying

$$\mathrm{supp}G^{\vee/\wedge} \subset \{x,y \ : \ x \in J^{\vee/\wedge}y)\}.$$

The Pauli-Jordan function:

$$G^{\mathrm{PJ}}(x,y) := G^{\vee}(x,y) - G^{\wedge}(x,y)$$

satisfies

$$\mathrm{supp}G^{\mathrm{PJ}} \subset \{x,y \ : \ x \in J(y)\}.$$

and can be used to solve the initial value problem of (13.2):

$$\begin{aligned} \phi(t,\vec{x}) = &-\int \partial_s G^{\mathrm{PJ}}(t,\vec{x},s,\vec{y})\Big|_{s=0}\phi(0,\vec{y})\mathrm{d}\vec{y} \\ &+\int G^{\mathrm{PJ}}(t,\vec{x},0,\vec{y})\pi(0,\vec{y})\mathrm{d}\vec{y}. \end{aligned} \tag{13.5}$$

Using (13.5) we obtain

$$\{\phi(x),\phi(y)\} = -G^{\mathrm{PJ}}(x-y).$$

The free (constant mass) field will be denoted by ϕ_{fr}, π_{fr}. We can use the same phase space $\mathcal{Y}_{\mathrm{KG}}$ for the free and perturbed scalar particle, identifying them for the initial condition at $t = 0$:

$$\phi_{\mathrm{fr}}(0,\vec{x}) = \phi(0,\vec{x}), \quad \pi_{\mathrm{fr}}(0,\vec{x}) = \pi(0,\vec{x}). \tag{13.6}$$

Thus we can introduce the plane wave functionals $a(k)$, $a^*(k)$ as in the free case, since they depend only on the Cauchy data at time 0.

We easily obtain the Hamiltonian density from the Lagrangian:

$$\mathcal{H}(x) = \frac{1}{2}\pi^2(x) + \frac{1}{2}\big(\vec{\partial}\phi(x)\big)^2 + \frac{1}{2}(m^2 + \kappa(x))\phi^2(x),$$

so that the full Hamiltonian generating the dynamics, first in the "Heisenberg picture" and then in the "Schrödinger picture", are

$$\begin{aligned} H(t) &= \int \mathcal{H}(t,\vec{x})\mathrm{d}\vec{x} \\ &= \int \Big(\frac{1}{2}\pi^2(t,\vec{x}) + \frac{1}{2}\big(\vec{\partial}\phi(t,\vec{x})\big)^2 + \frac{1}{2}(m^2 + \kappa(t,\vec{x}))\phi^2(t,\vec{x})\Big)\mathrm{d}\vec{x}, \quad (13.7) \\ H^{\mathrm{Sp}}(t) &= \int \Big(\frac{1}{2}\pi^2(\vec{x}) + \frac{1}{2}\big(\vec{\partial}\phi(\vec{x})\big)^2 + \frac{1}{2}(m^2 + \kappa(t,\vec{x}))\phi^2(\vec{x})\Big)\mathrm{d}\vec{x}, \quad (13.8) \end{aligned}$$

where $\phi(\vec{x}) = \phi(0,\vec{x})$, $\pi(\vec{x}) = \pi(0,\vec{x})$.

13.2 Dynamics in the interaction picture

The classical interaction picture Hamiltonian can be expressed in terms of plane wave functionals:

$$\begin{aligned} H_{\mathrm{Int}}(t) &= \frac{1}{2}\int \kappa(t,\vec{x})\phi^2_{\mathrm{fr}}(t,\vec{x})\mathrm{d}\vec{x} \quad (13.9) \\ &= \frac{1}{2}\int \frac{\mathrm{d}\vec{k}_1\mathrm{d}\vec{k}_2\kappa(t,\vec{k}_1+\vec{k}_2)}{(2\pi)^3\sqrt{2\varepsilon(\vec{k}_1)}\sqrt{2\varepsilon(\vec{k}_2)}}\Big(\mathrm{e}^{-\mathrm{i}t\varepsilon(\vec{k}_1)-\mathrm{i}t\varepsilon(\vec{k}_2)}a(-k_1)a(-k_2) \\ &\qquad +2\mathrm{e}^{\mathrm{i}t\varepsilon(\vec{k}_1)-\mathrm{i}t\varepsilon(\vec{k}_2)}a^*(k_1)a(-k_2) + \mathrm{e}^{\mathrm{i}t\varepsilon(\vec{k}_1)+\mathrm{i}t\varepsilon(\vec{k}_2)}a^*(k_1)a^*(k_2)\Big). \end{aligned}$$

We can also introduce the creation operators in the interaction picture:

$$a^*_t(k) := U_{\mathrm{Int}}(0,t)a^*(k)U_{\mathrm{Int}}(t,0). \quad (13.10)$$

They satisfy the equations generated by the Heisenberg picture interaction Hamiltonian $H^{\mathrm{Hp}}_{\mathrm{Int}}$:

$$\begin{aligned} H^{\mathrm{Hp}}_{\mathrm{Int}}(t) &= U_{\mathrm{Int}}(0,t)H_{\mathrm{Int}}(t)U_{\mathrm{Int}}(t,0) \quad (13.11) \\ &= \frac{1}{2}\int \frac{\mathrm{d}\vec{k}_1\mathrm{d}\vec{k}_2\kappa(t,\vec{k}_1+\vec{k}_2)}{(2\pi)^3\sqrt{2\varepsilon(\vec{k}_1)}\sqrt{2\varepsilon(\vec{k}_2)}}\Big(\mathrm{e}^{-\mathrm{i}t\varepsilon(\vec{k}_1)-\mathrm{i}t\varepsilon(\vec{k}_2)}a_t(-k_1)a_t(-k_2) \\ &\qquad +2\mathrm{e}^{\mathrm{i}t\varepsilon(\vec{k}_1)-\mathrm{i}t\varepsilon(\vec{k}_2)}a^*_t(k_1)a_t(-k_2) + \mathrm{e}^{\mathrm{i}t\varepsilon(\vec{k}_1)+\mathrm{i}t\varepsilon(\vec{k}_2)}a^*_t(k_1)a^*_t(k_2)\Big). \end{aligned}$$

We obtain

$$\begin{aligned}\dot{a}^*_t(k) &= \big\{a^*_t(k), H^{\mathrm{Hp}}_{\mathrm{Int}}(t)\big\}\\ &= \mathrm{i}\int \frac{\mathrm{d}\vec{k}_1\kappa(t,-\vec{k}+\vec{k}_1)}{(2\pi)^3\sqrt{2\varepsilon(\vec{k})}\sqrt{2\varepsilon(\vec{k}_1)}}\\ &\qquad\times\Big(\mathrm{e}^{-\mathrm{i}t\varepsilon(\vec{k})-\mathrm{i}t\varepsilon(\vec{k}_1)}a_t(-k_1)+\mathrm{e}^{-\mathrm{i}t\varepsilon(\vec{k})+\mathrm{i}t\varepsilon(\vec{k}_1)}a^*_t(k_1)\Big),\\ a^*_0(k) &= a^*(k).\end{aligned}$$

We obtain a symplectic evolution of the firm of the form

$$\begin{bmatrix} p_{t_+,t_-} & q_{t_+,t_-}\\ \overline{q_{t_+,t_-}} & \overline{p_{t_+,t_-}}\end{bmatrix} \tag{13.12}$$

more precisely,

$$\begin{bmatrix} a^*_{t_+}(k)\\ a_{t_+}(k)\end{bmatrix} = \int \mathrm{d}\vec{k}_1 \begin{bmatrix} p_{t_+,t_-}(k,k_1) & q_{t_+,t_-}(k,k_1)\\ \overline{q_{t_+,t_-}(k,k_1)} & \overline{p_{t_+,t_-}(k,k_1)}\end{bmatrix}\begin{bmatrix} a^*_{t_-}(k_1)\\ a_{t_-}(k_1)\end{bmatrix}.$$

(13.12) has a limit as $t_+, -t_- \to \infty$, which can be called the *classical scattering operator*.

One can try to solve the equations of motion by iterations. The first iteration is often (at least in the quantum context) called the *Born approximation*, and it gives the following formula for the elements of (13.12):

$$\begin{aligned}p^{\mathrm{Born}}_{t_+,t_-}(k,k_1) &= \delta(\vec{k}-\vec{k}_1)+\mathrm{i}\int_{t_-}^{t_+}\mathrm{d}s\frac{\kappa(s,-\vec{k}+\vec{k}_1)}{(2\pi)^3\sqrt{2\varepsilon(\vec{k})}\sqrt{2\varepsilon(\vec{k}_1)}}\mathrm{e}^{-\mathrm{i}s\varepsilon(\vec{k})+\mathrm{i}s\varepsilon(\vec{k}_1)},\\ q^{\mathrm{Born}}_{t_+,t_-}(k,k_1) &= \mathrm{i}\int_{t_-}^{t_+}\mathrm{d}s\frac{\kappa(s,-\vec{k}+\vec{k}_1)}{(2\pi)^3\sqrt{2\varepsilon(\vec{k})}\sqrt{2\varepsilon(\vec{k}_1)}}\mathrm{e}^{-\mathrm{i}s\varepsilon(\vec{k})-\mathrm{i}s\varepsilon(\vec{k}_1)}.\end{aligned}$$

13.3 Quantization

We are looking for quantum fields $\mathbb{R}^{1,3}\mapsto\hat{\phi}(x)$ satisfying

$$(-\Box+m^2)\hat{\phi}(x) = -\kappa(x)\hat{\phi}(x), \tag{13.13}$$

with the conjugate field $\hat{\pi}(x) := \dot{\hat{\phi}}(x)$ having the equal time commutators

$$\begin{aligned}[\hat{\phi}(t,\vec{x}),\hat{\phi}(t,\vec{y})] = [\hat{\pi}(t,\vec{x}),\hat{\pi}(t,\vec{y})] &= 0,\\ [\hat{\phi}(t,\vec{x}),\hat{\pi}(t,\vec{y})] &= \mathrm{i}\delta(\vec{x}-\vec{y}).\end{aligned} \tag{13.14}$$

and coinciding with the free field at time 0. The solution is given by putting "hats" onto (13.5):

$$\hat{\phi}(t,\vec{x}) = -\int \partial_s G^{\mathrm{PJ}}(t,\vec{x},s,\vec{y})\Big|_{s=0}\hat{\phi}(0,\vec{y})\mathrm{d}\vec{y} + \int G^{\mathrm{PJ}}(t,\vec{x},0,\vec{y})\hat{\pi}(0,\vec{y})\mathrm{d}\vec{y}. \tag{13.15}$$

Clearly,

$$[\hat{\phi}(x),\hat{\phi}(y)\} = -\mathrm{i}G^{\mathrm{PJ}}(x-y).$$

We would like to check whether the classical scattering operator and the classical dynamics are implementable in the Fock space for nonzero κ. By Thm **??**, we need to check the *Shale condition*, that is, whether the off-diagonal elements of (13.12) are square integrable. For simplicity, we will restrict ourselves to the Born approximation; the higher order terms do not change the conclusion.

The verification of the Shale condition is easier for the scattering operator. Consider

$$q^{\mathrm{Born}}_{\infty,-\infty}(k,k_1) = \mathrm{i}\int_{-\infty}^{\infty}\mathrm{d}s\frac{\kappa(s,-\vec{k}+\vec{k}_1)}{(2\pi)^3\sqrt{2\varepsilon(\vec{k})}\sqrt{2\varepsilon(\vec{k}_1)}}\mathrm{e}^{-\mathrm{i}s\varepsilon(\vec{k})-\mathrm{i}s\varepsilon(\vec{k}_1)}. \tag{13.16}$$

Recall that κ is a Schwartz function. Therefore, we can integrate by parts as many times as we want:

$$q^{\mathrm{Born}}_{\infty,-\infty}(k,k_1) = \mathrm{i}^{n+1}\int_{-\infty}^{\infty}\mathrm{d}s\frac{\partial_s^n\kappa(s,-\vec{k}+\vec{k}_1)}{(2\pi)^3\sqrt{2\varepsilon(\vec{k})}\sqrt{2\varepsilon(\vec{k}_1)}}\frac{\mathrm{e}^{-\mathrm{i}s\varepsilon(\vec{k})-\mathrm{i}s\varepsilon(\vec{k}_1)}}{\big(\varepsilon(\vec{k})+\varepsilon(\vec{k}_1)\big)^n}. \tag{13.17}$$

This decays in $\vec{k}$ and $\vec{k}_1$ as any inverse power, and hence is square integrable on $\mathbb{R}^3\times\mathbb{R}^3$. Therefore the classical scattering operator is implementable.

Next let us check the implementability of the dynamics, believing again that it is sufficient to check the Born approximation. We integrate by parts once:

$$\begin{aligned} & q^{\mathrm{Born}}_{t_+,t_-}(k,k_1) \\ = \;& \frac{-\kappa(t_+,-\vec{k}+\vec{k}_1)\mathrm{e}^{-\mathrm{i}t_+\varepsilon(\vec{k})-\mathrm{i}t_+\varepsilon(\vec{k}_1)}+\kappa(t_-,-\vec{k}+\vec{k}_1)\mathrm{e}^{-\mathrm{i}t_-\varepsilon(\vec{k})-\mathrm{i}t_-\varepsilon(\vec{k}_1)}}{(2\pi)^3\sqrt{2\varepsilon(\vec{k})}\sqrt{2\varepsilon(\vec{k}_1)}\big(\varepsilon(\vec{k})+\varepsilon(\vec{k}_1)\big)} \\ & +\int_{t_-}^{t_+}\mathrm{d}s\frac{\partial_s\kappa(s,-\vec{k}+\vec{k}_1)\mathrm{e}^{-\mathrm{i}s\varepsilon(\vec{k})-\mathrm{i}s\varepsilon(\vec{k}_1)}}{(2\pi)^3\sqrt{2\varepsilon(\vec{k})}\sqrt{2\varepsilon(\vec{k}_1)}\big(\varepsilon(\vec{k})+\varepsilon(\vec{k}_1)\big)}. \end{aligned} \tag{13.18}$$

Using that $\kappa(s,\vec{k}+\vec{k}_1)$ decays fast in the second variable, we see that (13.18) can be estimated by

$$\frac{C}{(\varepsilon(\vec{k})+\varepsilon(\vec{k}_1))^2},$$

which is square integrable. Therefore, the dynamics is implementable for any t_-, t_+.

By a similar computation we check that if we freeze $t_0 \in \mathbb{R}$, the dynamics generated by the momentary Hamiltonian $H_{\rm Int}(t_0)$ is implementable.

13.4 Quantum Hamiltonian

We would like to find a time-dependent Hamiltonian $\hat{H}(t)$ such that

$$\hat{\phi}(t,\vec{x}) = \mathrm{Texp}\left(-\mathrm{i}\int_0^t \hat{H}(s)\mathrm{d}s\right)^{-1} \hat{\phi}(0,\vec{x})\mathrm{Texp}\left(-\mathrm{i}\int_0^t \hat{H}(s)\mathrm{d}s\right). \qquad (13.19)$$

Formally, the quantum Hamiltonians, first in the Heisenberg, then in the Schrödinger picture, are given by

$$\hat{H}^{\rm Hp}(t) := \int \Big(\frac{1}{2}\hat{\pi}^2(t,\vec{x}) + \frac{1}{2}\big(\vec{\partial}\hat{\phi}(t,\vec{x})\big)^2 + \frac{1}{2}(m^2+\kappa(t,\vec{x}))\hat{\phi}^2(t,\vec{x})\Big)\mathrm{d}\vec{x}, \quad (13.20)$$

$$\hat{H}(t) := \int \Big(\frac{1}{2}\hat{\pi}^2(\vec{x}) + \frac{1}{2}\big(\vec{\partial}\hat{\phi}(\vec{x})\big)^2 + \frac{1}{2}(m^2+\kappa(t,\vec{x}))\hat{\phi}^2(\vec{x})\Big)\mathrm{d}\vec{x}. \qquad (13.21)$$

We will treat the Schrödinger picture Hamiltonian, that is (13.21), as the standard one. It is expressed in terms of zero time fields. It is clear that it is ill-defined. One could improve it by putting $:\cdots:$, that is by the Wick ordering. We will see later on that even the Wick-ordered expression (13.21) does not define an operator.

Formally (13.47) remains true if we add a time dependent constant $C(t)$ to (13.21). We will see that in order to define correct Hamiltonians $\hat{H}(t)$ this constant has to be infinite, even after Wick ordering. We will obtain bounded from below Hamiltonians $\hat{H}_{\rm ren}(t)$, however the vacuum will not be contained in their form domain. Therefore, the condition $(\Omega|\hat{H}_{\rm ren}(t)\Omega) = 0$ for all t, which is equivalent to the Wick ordering, cannot be imposed.

The interaction Hamiltonian is formally given by

$$\hat{H}_{\rm Int}(t) = \frac{1}{2}\int \kappa(t,\vec{x})\hat{\phi}^2_{\rm fr}(t,\vec{x})\mathrm{d}\vec{x}, \qquad (13.22)$$

$$\hat{\phi}_{\rm fr}(x) = \int \frac{\mathrm{d}\vec{k}}{\sqrt{(2\pi)^3}\sqrt{2\varepsilon(\vec{k})}}\left(\mathrm{e}^{-\mathrm{i}t\varepsilon(\vec{k})+\mathrm{i}\vec{k}\vec{x}}\hat{a}(k) + \mathrm{e}^{\mathrm{i}t\varepsilon(\vec{k})-\mathrm{i}\vec{k}\vec{x}}\hat{a}^*(k)\right), \qquad (13.23)$$

where (13.23) is taken from (8.58). Here is the Wick ordered interaction Hamiltonian:

$$\begin{aligned} :\hat{H}_{\rm Int}(t): \;=\; & \frac{1}{2}\int \frac{\mathrm{d}\vec{k}_1\mathrm{d}\vec{k}_2\kappa(t,\vec{k}_1+\vec{k}_2)}{(2\pi)^3\sqrt{2\varepsilon(\vec{k}_1)}\sqrt{2\varepsilon(\vec{k}_2)}}\Big(\mathrm{e}^{-\mathrm{i}t\varepsilon(\vec{k}_1)-\mathrm{i}t\varepsilon(\vec{k}_2)}\hat{a}(-k_1)\hat{a}(-k_2) \\ & +2\mathrm{e}^{\mathrm{i}t\varepsilon(\vec{k}_1)-\mathrm{i}t\varepsilon(\vec{k}_2)}\hat{a}^*(k_1)\hat{a}(-k_2) + \mathrm{e}^{\mathrm{i}t\varepsilon(\vec{k}_1)+\mathrm{i}t\varepsilon(\vec{k}_2)}\hat{a}^*(k_1)\hat{a}^*(k_2)\Big). \end{aligned}$$

where $\kappa(t,\vec{k})$ is a partial Fourier transform of $\kappa(t,\vec{x})$.

13.5 The vacuum energy

We would like to compute

$$\mathrm{e}^{-\mathrm{i}\mathcal{E}} := (\Omega|\hat{S}\Omega) = \Big(\Omega|\mathrm{Texp}\Big(-\int \mathrm{i}\hat{H}_{\mathrm{Int}}(t)\mathrm{d}t\Big)\Omega\Big). \tag{13.24}$$

Not surprisingly, (13.24) will require a renormalization. So eventually we will compute its renormalized version:

$$\mathrm{e}^{-\mathrm{i}\mathcal{E}^{\mathrm{ren}}} := (\Omega|\hat{S}^{\mathrm{ren}}\Omega) = \Big(\Omega|\mathrm{Texp}\Big(-\int \mathrm{i}\hat{H}^{\mathrm{ren}}_{\mathrm{Int}}(t)\mathrm{d}t\Big)\Omega\Big). \tag{13.25}$$

Anyway, we treat (13.24) as the starting point of our computations. The path integrals approach leads to the following expression for (13.24) in terms of Gaussian integrals:

$$\mathrm{e}^{-\mathrm{i}\mathcal{E}} = \frac{\int \exp(\mathrm{i}\int \mathcal{L}(x,\phi,\phi_\mu)\mathrm{d}x)\mathrm{D}\phi}{\int \exp(\mathrm{i}\int \mathcal{L}_0(x,\phi,\phi_\mu)\mathrm{d}x)\mathrm{D}\phi}, \tag{13.26}$$

where the Lagrangians are

$$\begin{aligned}\mathcal{L}(x) =& -\frac{1}{2}\partial_\mu\phi(x)\partial^\mu\phi(x) - \frac{1}{2}(m^2+\kappa(x))\phi(x)^2,\\ \mathcal{L}_0(x) =& -\frac{1}{2}\partial_\mu\phi(x)\partial^\mu\phi(x) - \frac{1}{2}m^2\phi(x)^2,\end{aligned}$$

and we use the Minkowski signature $x = (x^0,\dots,x^3)$. (13.26) can be evaluated as

$$\mathcal{E} = -\frac{\mathrm{i}}{2}\mathrm{Tr}\Big(\ln(-\Box + m^2 + \kappa - \mathrm{i}0) - \ln(-\Box + m^2 - \mathrm{i}0)\Big). \tag{13.27}$$

It is much more convenient to do computations in the Euclidean setting. Various symbols from the Euclidean case will be decorated by the subscript E. In particular, the Euclidean version of the path integrals becomes

$$\mathrm{e}^{-\mathcal{E}^{\mathrm{E}}} = \frac{\int \exp(-\int \mathcal{L}^{\mathrm{E}}(x,\phi,\phi_\mu)\mathrm{d}x)\mathrm{D}\phi}{\int \exp(-\int \mathcal{L}^{\mathrm{E}}_0(x,\phi,\phi_\mu)\mathrm{d}x)\mathrm{D}\phi}, \tag{13.28}$$

where the Euclidean Lagrangians are

$$\begin{aligned}\mathcal{L}^{\mathrm{E}}(x) =& \frac{1}{2}\partial_\mu\phi(x)\partial^\mu\phi(x) + \frac{1}{2}(m^2+\kappa(x))\phi(x)^2,\\ \mathcal{L}^{\mathrm{E}}_0(x) =& \frac{1}{2}\partial_\mu\phi(x)\partial^\mu\phi(x) + \frac{1}{2}m^2\phi(x)^2,\end{aligned}$$

and we use the Euclidean signature $x = (x^1,\dots,x^4)$. We have

$$\mathrm{e}^{-\mathcal{E}^{\mathrm{E}}} = \Big(\det(\hat{p}^2+m^2+\kappa)(\hat{p}^2+m^2)^{-1}\Big)^{-\frac{1}{2}}, \tag{13.29}$$

$$\mathcal{E}^{\mathrm{E}} = \frac{1}{2}\mathrm{Tr}\Big(\ln(\hat{p}^2+m^2+\kappa) - \ln(\hat{p}^2+m^2)\Big), \tag{13.30}$$

where $\hat{p}^2$ is the 4-dimensional Laplacian.

As we computed in Subsection 12.2, $\mathcal{E}^{\mathrm{E}}$ needs to be renormalized and equals (see (12.35)):

$$\mathcal{E}^{\mathrm{E,ren}} = \mathcal{E}_2^{\mathrm{E,ren}} + \sum_{n=3}^{\infty} \mathcal{E}_n^{\mathrm{E}}, \tag{13.31}$$

$$\mathcal{E}_2^{\mathrm{E,ren}} = -\int |\kappa(k)|^2 \frac{\mathrm{d}k}{(2\pi)^4} \pi^{\mathrm{E,ren}}(k^2), \tag{13.32}$$

$$\pi^{\mathrm{E,ren}}(k^2) = \frac{1}{4(4\pi)^2}\Big(\frac{1}{\theta}\log\frac{1+\theta}{1-\theta} - 2\Big), \qquad \theta = \sqrt{\frac{k^2}{k^2+4m^2}}. \tag{13.33}$$

We would like to find the Minkowskian analogs of $\mathcal{E}^{\mathrm{E}}$ and $\mathcal{E}_2^{\mathrm{E}}$:

$$\mathcal{E} = \mathcal{E}_2^{\mathrm{ren}} + \sum_{n=2}^{\infty} \mathcal{E}_n, \tag{13.34}$$

$$\mathcal{E}_2^{\mathrm{ren}} = \int |\kappa(k)|^2 \frac{\mathrm{d}k}{(2\pi)^4} \pi^{\mathrm{ren}}(k^2). \tag{13.35}$$

The Wick rotation consists in replacing x^4 with $\mathrm{i}x^0$ everywhere except for $\kappa(x)$, where we do not change anything. More precisely, we replace x^4 with zx^0, where z is a complex parameter which is continued as $\mathrm{e}^{\mathrm{i}\alpha}$ with $\alpha \in [0, \frac{\pi}{2}]$. Thus the Euclidean quantities are treated as functions $F(z)$, where $F(z)\big|_{z=1}$ is the Euclidean value and $F(z)\big|_{z=\mathrm{i}}$ the Wick rotated value.

This implies replacing p^4 with $-\mathrm{i}p^0$. Moreover, the Euclidean x^2 and p^2 are replaced with Minkowskian $x^2 + \mathrm{i}0$ and $p^2 - \mathrm{i}0$. The Euclidean Lebesgue measures $\mathrm{d}x$ and $\mathrm{d}k$ are replaced in the Minkowski space by $\mathrm{i}\mathrm{d}x$, resp. $-\mathrm{i}\mathrm{d}k$. Consequently, the Euclidean action $\int \mathcal{L}^{\mathrm{E}}(x,\phi,\phi_{,\mu})\mathrm{d}x$ becomes after the Wick rotation $-\mathrm{i}\int \mathcal{L}(x,\phi,\phi_{,\mu})\mathrm{d}x$. Thus $\mathrm{e}^{-\mathcal{E}^{\mathrm{E}}}(z)\big|_{z=\mathrm{i}} = \mathrm{e}^{-\mathrm{i}\mathcal{E}}$, and consequently

$$\mathcal{E} = -\mathrm{i}\mathcal{E}^{\mathrm{E}}(z)\big|_{z=\mathrm{i}} \tag{13.36}$$

$$\begin{aligned}\mathcal{E}_2 &= -\mathrm{i}\mathcal{E}_2^{\mathrm{E,ren}}(z)\big|_{z=\mathrm{i}} = -\mathrm{i}\Big(-\int |\kappa(k)|^2 \frac{(-\mathrm{i})\mathrm{d}k}{(2\pi)^4} \pi^{\mathrm{E,ren}}(k^2 - \mathrm{i}0)\Big) \\ &= \int |\kappa(k)|^2 \frac{\mathrm{d}k}{(2\pi)^4} \pi^{\mathrm{E,ren}}(k^2 - \mathrm{i}0).\end{aligned} \tag{13.37}$$

Thus comparing with (13.35) we obtain

$$\pi^{\mathrm{ren}}(k^2) = \pi^{\mathrm{E,ren}}(k^2 - \mathrm{i}0). \tag{13.38}$$

Taking into account (13.33), we obtain

$$\pi^{\rm ren}(k^2) = \frac{1}{4(4\pi)^2}\Big(\frac{1}{\theta}\log\frac{1+\theta}{1-\theta} - 2\Big), \qquad \theta = \frac{\sqrt{k^2}}{\sqrt{k^2+4m^2}}, \quad 0 < k^2; \quad (13.39)$$

$$= \frac{1}{4(4\pi)^2}\Big(\frac{2}{\theta}\arctan\theta - 2\Big), \qquad \theta = \frac{\sqrt{-k^2}}{\sqrt{k^2+4m^2}}, \quad -4m^2 < k^2 < 0; \quad (13.40)$$

$$= \frac{1}{4(4\pi)^2}\Big(\frac{1}{\theta}\Big(\log\frac{\theta+1}{\theta-1} - \mathrm{i}\pi\Big) - 2\Big), \qquad \theta = \frac{\sqrt{-k^2}}{\sqrt{-k^2-4m^2}}, \quad k^2 < -4m^2. \quad (13.41)$$

Here is the calculation. First we assume that $k^2 > 0$. Then we just take the Euclidean value. Then we use analytic continuation, remembering that k^2 may have negative imaginary part. As k^2 decreases, $\theta := \frac{\sqrt{k^2}}{\sqrt{k^2+4m^2}}$ first varies from 1 to 0, then from 0 to $-\mathrm{i}\infty$, finally, from ∞ to 1. Therefore, $\frac{1+\theta}{1-\theta}$ first varies from ∞ to 1, then goes over the lower semicircle, finally, from -1 to $-\infty$. Next we use $\log\frac{1+\mathrm{i}y}{1-\mathrm{i}y} = 2\mathrm{i}\arctan y$, and for $y < 0$, $\log(y - \mathrm{i}0) = \log|y| - \mathrm{i}\pi$.

(13.39) corresponds to a spatial transfer of energy-momentum. In (13.40) the transfer is time-like, but the energy is below the 2-particle threshold. In (13.41) it is above this threshold, and $\pi^{\rm ren}$ acquires a nonzero imaginary part responsible for the decay of the vacuum.

Here are operator-theoretic formulas for the renormalized vacuum energies:

$$\mathcal{E}_2^{\rm ren} = -\frac{\mathrm{i}}{4}\mathrm{Tr}\Big(\big(\kappa(x)(-\Box + m^2 - \mathrm{i}0)^{-1}\big)^2 - \kappa(x)^2(-\Box + m^2 - \mathrm{i}0)^{-2}\Big),$$

$$\mathcal{E}^{\rm ren} = -\frac{\mathrm{i}}{2}\mathrm{Tr}\Big(\log\big(\mathbb{1} + \kappa(x)(-\Box + m^2 - \mathrm{i}0)^{-1}\big) - \kappa(x)(-\Box + m^2 - \mathrm{i}0)^{-1} + \frac{1}{2}\kappa^2(x)(-\Box + m^2 - \mathrm{i}0)^{-2}\Big). \quad (13.42)$$

13.6 Renormalized scattering operator and Hamiltonian

The naive Hamiltonian $\hat{H}(t)$ and the naive scattering operator $\hat{S}$ are ill defined. However, in $\hat{S}$ only the overall coefficient is ill defined. We can renormalize $\hat{S}$ by multiplying it by a divergent phase:

$$\hat{S}^{\rm ren} \quad = \quad \mathrm{e}^{\mathrm{i}C\int\kappa(x)\mathrm{d}x + \mathrm{i}\pi(0)\int\kappa(x)^2\mathrm{d}x}\hat{S}, \quad (13.43)$$

where C is the constant responsible for the Wick ordering and $\pi(0)$ is the 2nd order renormalization. Note that both infinite quantities are quite well behaved – they depends locally on the interaction, and therefore the renormalization preserves the Einstein causality. This manifests itself in the identity

$$\hat{S}^{\rm ren}(\kappa_2)\hat{S}^{\rm ren}(\kappa_1) = \hat{S}^{\rm ren}(\kappa_2 + \kappa_1), \quad (13.44)$$

whenever $\mathrm{supp}\kappa_2$ is later than $\mathrm{supp}\kappa_1$.

If we cut off the perturbation in time by setting $\kappa_{t_+,t_-}(x) := \mathbb{1}_{[t_-,t_+]}(x^0)\kappa(x)$, then we can repeat the same constructions, obtaining the renormalized scattering operator $\hat{S}^{\rm ren}(t_2,t_1)$. For $t_3 > t_2 > t_1$, as a special case of (13.44), we

have

$$\hat{S}^{\rm ren}(t_3,t_2)\hat{S}^{\rm ren}(t_2,t_1)=\hat{S}^{\rm ren}(t_3,t_1). \tag{13.45}$$

Thus we get a unitary evolution given by

$$U^{\rm ren}(t_+,t_-):={\rm e}^{-{\rm i}t_+H_0}\hat{S}^{\rm ren}(t_+,t_-){\rm e}^{{\rm i}t_-H_0}. \tag{13.46}$$

Its generator will be called $\hat{H}^{\rm ren}(t)$, so that

$$\hat{\phi}(t,\vec{x})={\rm Texp}\left(-{\rm i}\int_0^t\hat{H}^{\rm ren}(s){\rm d}s\right)^{-1}\hat{\phi}(0,\vec{x}){\rm Texp}\left(-{\rm i}\int_0^t\hat{H}^{\rm ren}(s){\rm d}s\right), \tag{13.47}$$

Formally, we can write for the Hamiltonian and Lagrangian density

$$\begin{aligned}\hat{H}^{\rm ren}(t) &= \hat{H}(t)-\pi(0)\int\kappa(t,\vec{x})^2{\rm d}\vec{x}-C\int\kappa(t,\vec{x}){\rm d}\vec{x}, &(13.48)\\ \mathcal{L}^{\rm ren}(x) &= \mathcal{L}(x)+\frac{1}{2}\pi(0)\kappa(x)^2+\frac{1}{2}C\kappa(x). &(13.49)\end{aligned}$$