

**Lecture 5: BOSONS: FROM NON-RELATIVISTIC TO
RELATIVISTIC QUANTUM FIELD THEORY**

Having set up a suitable formalism, we now study more generally, quantum boson systems in the so-called **second quantization formulation**.

In the preceding lecture, we have assumed that bosons can occupy only a finite number of quantum states, for example, because only spin degrees of freedom are relevant or because bosons live on a finite space lattice.

In this lecture, the available states belong themselves to a Hilbert space. The simplest application is Bose–Einstein condensation for a system of independent bosons.

In the presence of interactions, the **holomorphic formalism** leads to a description of the **Bose gas** in the grand canonical formulation in terms of a **non-relativistic quantum field theory**. One application is the Helium superfluid phase transition.

Replacing in the action the non-relativistic by the relativistic kinematics and enforcing **locality**, we construct a relativistic quantum field theory for a **neutral scalar boson field**.

Then, we begin our study of **local, relativistic quantum field theory**.

It is convenient to describe its properties first in **real time**, before returning to the euclidean formalism because some aspects, like the relation between fields and particles, are easier to understand. Various expressions for the scattering S -matrix follow.

5.1 Bose–Einstein condensation

We first discuss the example of a system of independent bosons. Of course, in such a case the sophisticated formalism that we have set-up in section 4.10 is not really required. But the application to this simple situation will give us an opportunity to explain **Bose–Einstein condensation** and provide us with a transition to section 5.2. It will lead us to generalize the holomorphic formalism from finite vector space to Hilbert space.

In the case of independent particles, the partition function factorizes into a product of partition functions of harmonic oscillators corresponding to each energy level, a result that also follows directly from the path integral representation (4.59).

5.1.1 Independent bosons: the equation of state

In the absence of interactions, using the partition function or directly equation (4.61) (see section 4.10.2), the average occupation number is given by

$$\langle \mathbf{N} \rangle = \sum_i \langle n_i \rangle, \quad \langle n_i \rangle = \langle z_i(0) \bar{z}_i(0) \rangle$$

where $\langle n_i \rangle$ is the average occupation number of the state i with energy ω_i .

Since the bosons do not interact, the two-point function for state i is just related to the corresponding harmonic oscillator $\mathbf{H}_0(\omega_i) - \mu \mathbf{N}$, where μ is the chemical potential (equation (4.35)):

$$\langle \bar{z}_i(t) z_j(0) \rangle = \delta_{ij} \Delta_i(t) = \delta_{ij} e^{-(\omega_i - \mu)t} \left(\theta(t) + \frac{1}{e^{\beta(\omega_i - \mu)} - 1} \right).$$

For $t = 0$, setting $\theta(0) = 0$ (normal order), one obtains the equation of state

$$\langle \mathbf{N} \rangle = \sum_i \frac{1}{e^{\beta(\omega_i - \mu)} - 1}, \quad (5.1)$$

This expression can also be expressed in terms of the one-particle Hamiltonian $H^{(1)}$ with spectrum ω_i as

$$\langle \mathbf{N} \rangle = \text{tr} \frac{1}{e^{\beta(H^{(1)} - \mu)} - 1}. \quad (5.2)$$

Note that these expressions are defined only for $\mu < \inf_i \omega_i$. Moreover, $\langle \mathbf{N} \rangle$ is an increasing function of μ and diverges for $\mu \rightarrow \inf_i \omega_i$.

5.1.2 From finite-dimensional vector space to Hilbert space: the harmonic potential

Up to now, we have assumed that the one-particle states belong to a finite-dimensional vector space. We now generalize the formalism to the situation where **one-particle states belong themselves to a Hilbert space**. We discuss this situation more systematically in section 5.2 but, here, as an introduction, we study the equation of state of a system of independent particles. The formal expression (5.2) is still valid, but $H^{(1)}$ is then a one-particle Hamiltonian operator.

Harmonic potential in the semi-classical limit. We first consider the example of particles in an isotropic harmonic well in d -dimensional space. The one-particle quantum Hamiltonian can be written as

$$H^{(1)}(\hat{\mathbf{p}}, \hat{\mathbf{q}}) = \frac{1}{2m} \hat{\mathbf{p}}^2 + \frac{1}{2} m \omega^2 \hat{\mathbf{q}}^2.$$

The average number of particles at high temperature (high compared to the separation $\hbar\omega$ between energy levels and thus for $\beta\hbar\omega \ll 1$) is given as an integral over phase space by the semi-classical expression

$$\langle \mathbf{N} \rangle \sim \frac{1}{(2\pi\hbar)^d} \int \frac{d^d p \, d^d q}{e^{\beta(H^{(1)}(\mathbf{p}, \mathbf{q}) - \mu)} - 1}. \quad (5.3)$$

In the semi-classical approximation, $\langle \mathbf{N} \rangle$ is not defined for $\mu > 0$. For $\mu < 0$ the average number of particles is still an increasing function of μ .

We then note that for $d > 1$ the integral has a finite limit for $\mu = 0$, which can be calculated explicitly. One finds,

$$\langle \mathbf{N} \rangle = \zeta(d) / (\hbar\omega\beta)^d, \quad (5.4)$$

where ζ is the Riemann function.

This result leads to an apparent paradox: by decreasing the temperature at fixed average number of particles, one encounters a limiting temperature

$$T_c = \frac{1}{\beta_c} = \hbar\omega \left(\frac{\langle \mathbf{N} \rangle}{\zeta(d)} \right)^{1/d}.$$

At first instance, this phenomenon reflects a limitation of the semi-classical approximation since, for a Hamiltonian with a discrete spectrum, or at least a gap, $\langle \mathbf{N} \rangle$ diverges when μ tends toward the ground state energy.

However, let us examine more closely what happens for energy levels close to the ground state.

At β or $T = T_c$ fixed, we increase $\langle \mathbf{N} \rangle$ by a macroscopic amount δN , that is, $\delta N = O(\langle \mathbf{N} \rangle) = O((\hbar\omega\beta)^{-d})$. The chemical potential then tends toward the ground state energy $E_0 = d\hbar\omega/2$.

For all states other than the ground state, the energy E satisfies $E - \mu \geq E - E_0 \geq \hbar\omega$ and this bounds the individual occupation numbers since

$$n \leq \frac{1}{e^{\beta\hbar\omega} - 1} = O(1/\beta\hbar\omega) \ll \delta N = O((\hbar\omega\beta)^{-d}).$$

Therefore, these states can absorb only a negligible fraction of the increase, and the sum of all corresponding occupation numbers is still given by equation (5.4). By contrast, for the ground state the equation

$$\delta N \sim \frac{1}{e^{\beta(E_0 - \mu)} - 1} \sim \frac{1}{\beta(E_0 - \mu)}$$

has the solution

$$\beta(E_0 - \mu) = \frac{1}{\delta N} = O((\hbar\omega\beta)^d) \ll \hbar\omega\beta.$$

For space dimensions larger than one, one thus observes a remarkable phenomenon characteristic of bosons: at fixed average number of particles, below T_c a macroscopic fraction of the gas occupies only one quantum state, the ground state of the one-particle Hamiltonian. This is the essence of the physical phenomenon called Bose–Einstein condensation and T_c is the condensation temperature.

5.1.3 Free Bose gas in a box

We now consider free identical bosons of mass m confined in a box of equal size L in all dimensions and, thus, of volume L^d in dimension d . The one-particle quantum Hamiltonian is simply the free Hamiltonian

$$H^{(1)} = \hat{\mathbf{p}}^2 / 2m .$$

In a box, momenta are quantized with the precise form depending on the boundary conditions. Assuming periodic boundary conditions for convenience, but this plays no role in the analysis, one finds

$$\mathbf{p} = 2\pi\hbar \mathbf{n} / L , \quad \mathbf{n} \in \mathbb{Z}^d .$$

In the infinite volume limit $L \rightarrow \infty$, the system always ends up here in a **high temperature** situation, since the splitting between neighbouring energies decreases as $\hbar^2 / 2mL^2$.

The equation of state, limit of equation (5.1) where sums are replaced by integrals, in d space dimensions takes a form analogous to equation (5.3):

$$\langle \mathbf{N} \rangle \sim \frac{1}{(2\pi\hbar)^d} \int \frac{d^d p d^d q}{e^{\beta(\mathbf{p}^2/2m - \mu)} - 1}.$$

The integration over \mathbf{q} yields a factor L^d and, thus, the density is given by

$$\rho(\beta, \mu) = \frac{\langle \mathbf{N} \rangle}{L^d} \underset{L \rightarrow \infty}{\sim} \frac{1}{(2\pi\hbar)^d} \int \frac{d^d p}{e^{\beta(\mathbf{p}^2/2m - \mu)} - 1}. \quad (5.5)$$

One notes that this expression not defined for $\mu > 0$ and that for $d > 2$ ρ , which is an increasing function of μ , is bounded by

$$\rho_c = \frac{1}{(2\pi\hbar)^d} \int \frac{d^d p}{e^{\beta\mathbf{p}^2/2m} - 1} = \zeta(d/2)/\chi^d,$$

where $\zeta(z)$ is the Riemann function, and χ the thermal wave length:

$$\chi = 2\pi\hbar\sqrt{m/\beta} = 2\pi\hbar/\sqrt{mT}.$$

Alternatively, at ρ fixed, the equation of state has no solution for temperatures $T < T_c(\rho) \propto (\hbar^2/m)\rho^{2/d}$. Returning to a box of finite size, in which momenta are quantized and energy levels discrete (as in equation (5.1)), one verifies that the remaining particles accumulate in the ground state, here the state with zero momentum. This provides another realization of Bose–Einstein condensation.

Finally, note that the **chemical potential is not directly a physical observable** and is generally eliminated in favour of the gas pressure $P = \ln \mathcal{Z} / \beta L^d$.

Remark. Thrice, we have used implicitly the identity

$$\int_0^\infty \frac{ds s^{\alpha-1}}{e^s - 1} = \Gamma(\alpha)\zeta(\alpha)$$

which can, for example, be proved by expanding

$$\frac{1}{e^s - 1} = \sum_{n=1}^\infty e^{-ns},$$

integrating each term and summing.

5.2 Generalized path integrals: the quantum Bose gas

In this section, we show how a natural generalization of the path integral formalism presented in sections 4.9 and 4.10 allows deriving a functional or field integral representation (one integrates over classical fields) of the partition function for non-relativistic boson systems.

We again consider the thermodynamic properties of a system of particles obeying the Bose statistics, in the **grand canonical** formulation.

5.2.1 Fock space

To show how functional methods can be used in this context, we proceed in several steps.

We denote by $\psi_n(x_1, \dots, x_n)$, $x_i \in \mathbb{R}^d$, the wave function describing a system of n identical bosons (assumed without other quantum numbers), a function thus invariant under permutation of its n arguments.

We then introduce a complex function (a field) $\varphi(x)$ (which generalizes the complex vector z_i of section 4.9) and the functional

$$\Psi(\varphi) = \sum_{n=0}^{\infty} \frac{1}{n!} \left(\int \prod_i d^d x_i \varphi(x_i) \right) \psi_n(x_1, \dots, x_n). \quad (5.6)$$

Because the wave functions are symmetric, $\Psi(\varphi)$ is a generating functional of the wave functions (see section 3.6.2). The constant ψ_0 is the coefficient of the empty state or vacuum.

The vector space of generating functionals is then endowed with a scalar product, which takes the form of a generalized path integral, a **functional** or **field integral**, because it involves integrating over complex fields $\varphi(x), \bar{\varphi}(x)$. The scalar product of Ψ_1 generating functions $\{\psi_n^{(1)}\}$ and Ψ_2 generating functions $\{\psi_n^{(2)}\}$ is given by

$$(\Psi_1, \Psi_2) = \int [d\varphi d\bar{\varphi}] \overline{\Psi_1(\varphi)} \Psi_2(\varphi) \exp \left[- \int d^d x \bar{\varphi}(x) \varphi(x) \right]. \quad (5.7)$$

The integral is implicitly normalized by the condition

$$(\Psi \equiv 1, \Psi \equiv 1) = 1 = \int [d\varphi d\bar{\varphi}] \exp \left[- \int d^d x \bar{\varphi}(x) \varphi(x) \right].$$

The complex vector space of functionals with finite norm is called a **Fock space**.

Since the scalar product is given by a Gaussian integral, to calculate scalar products one only needs the two-point function. It can be derived from the general integral

$$\mathcal{J}(J, \bar{J}) = \int [d\varphi d\bar{\varphi}] \exp \left\{ \int d^d x \left[-\bar{\varphi}(x) \varphi(x) + J(x) \bar{\varphi}(x) + \bar{J}(x) \varphi(x) \right] \right\}.$$

Translating the field and using the normalization condition, one obtains

$$\mathcal{J}(J, \bar{J}) = \exp \left[\int d^d x \bar{J}(x) J(x) \right].$$

Functional differentiation with respect to J, \bar{J} then yields the two-point function, ($\delta^{(d)}$ is the d -dimensional Dirac-function)

$$\int [d\varphi d\bar{\varphi}] \bar{\varphi}(x_1)\varphi(x_2) \exp \left[- \int d^d x \bar{\varphi}(x)\varphi(x) \right] = \delta^{(d)}(x_1 - x_2).$$

Using Wick's theorem, one obtains the norm of the functional (5.6):

$$|\Psi|^2 = (\Psi, \Psi) = \sum_{n=0} \frac{1}{n!} \left(\int \prod_i d^d x_i \right) |\psi_n(x_1, \dots, x_n)|^2.$$

The Fock space is the space of functionals with **finite norm**. When $|\Psi|^2 = 1$, the n th term in the sum gives the probability to find bosons in an n -particle state.

5.2.2 Hamiltonians in Fock space

We consider the Hamiltonian of a quantum Bose gas, in d space dimensions, of the form

$$\mathbf{H} = \mathbf{T} + \mathbf{V}, \quad (5.8)$$

where \mathbf{T} is the kinetic term, which in the sub-space of n -particle wave functions is represented by

$$T_n = -\frac{\hbar^2}{2m} \sum_{i=1}^n \nabla_{x_i}^2 \quad (5.9)$$

and \mathbf{V} is a pair interaction represented by

$$V_n = \sum_{i < j \leq n} V(x_i - x_j) \quad \text{with} \quad V(x) = V(-x). \quad (5.10)$$

For simplicity, we do not introduce here a one-particle potential.

We then introduce the formalism described in sections 4.9 and 4.10.

Hamiltonian representation. The kinetic term and the pair potential can be represented as operators acting on elements of Fock's space of the form (5.6).

To derive the representation of the kinetic term \mathbf{T} , one starts from the identity

$$\begin{aligned} & \int d^d x \varphi(x) \nabla_x^2 \frac{\delta}{\delta \varphi(x)} \Psi(\varphi) \\ &= \int d^d x \varphi(x) \nabla_x^2 \sum_n \frac{1}{(n-1)!} \int \left(\prod_{i < n} d^d x_i \varphi(x_i) \right) \psi_n(x_1, \dots, x_{n-1}, x). \end{aligned}$$

In the right hand side the argument x can be renamed x_n , and the coefficient of $\prod_{i \leq n} \varphi(x_i)$ can then be symmetrized. This generates a factor $1/n$ and yields the sum of all second derivatives, which is proportional to the kinetic term (5.9). Thus,

$$[\mathbf{T}\Psi](\varphi) = -\frac{\hbar^2}{2m} \int d^d x \varphi(x) \nabla_x^2 \frac{\delta}{\delta \varphi(x)} \Psi(\varphi).$$

Similarly, one verifies that the two-body potential \mathbf{V} , which in the n -particle subspace is given by (5.10), can be generated by differentiating twice with respect to φ with two different arguments. One finds

$$[\mathbf{V}\Psi](\varphi) = \frac{1}{2} \int d^d x d^d y \varphi(x)\varphi(y)V(x-y) \frac{\delta^2}{\delta\varphi(x)\delta\varphi(y)} \Psi(\varphi).$$

We have derived a representation of the total Hamiltonian $\mathbf{H} = \mathbf{T} + \mathbf{V}$ when acting on Fock's space. Finally, the representation of the particle number operator is simply

$$\mathbf{N} = \int d^d x \varphi(x) \frac{\delta}{\delta\varphi(x)} \quad \text{and} \quad [\mathbf{N}, \mathbf{H}] = 0.$$

For reasons already explained in section 4.10, one considers, in what follows, the modified Hamiltonian $\mathbf{H} - \mu\mathbf{N}$, where the chemical potential μ is a parameter that allows varying the average occupation number $\langle \mathbf{N} \rangle$.

5.2.3 Kernels

Following the method of sections 4.9, one can derive the kernel representation of operators. The complex variables z_i of the holomorphic representation (section 4.3) are replaced by $\varphi(x)$ where the continuum coordinate x plays the role of the indices i . We denote by $\bar{\varphi}(x)$ the field conjugate to $\varphi(x)$.

One verifies that the kernel representation of the identity associated with the scalar product (5.7) reads (see also equation (4.18))

$$\mathcal{I}(\varphi, \bar{\varphi}) = \exp \left[\int d^d x \bar{\varphi}(x) \varphi(x) \right].$$

The kernel representation of the Hamiltonian is then

$$\begin{aligned} \langle \varphi | \mathbf{H} | \bar{\varphi} \rangle &= \mathcal{I}(\varphi, \bar{\varphi}) \\ &\times \left[-\frac{\hbar^2}{2m} \int d^d x \varphi(x) \nabla_x^2 \bar{\varphi}(x) + \frac{1}{2} \int d^d x d^d y \varphi(x) \varphi(y) V(x-y) \bar{\varphi}(x) \bar{\varphi}(y) \right]. \end{aligned}$$

The particle number operator is represented by

$$\langle \varphi | \mathbf{N} | \bar{\varphi} \rangle = \mathcal{I}(\varphi, \bar{\varphi}) \int d^d x \bar{\varphi}(x) \varphi(x).$$

5.3 Partition function: the field integral representation

A representation of matrix elements of the statistical operator can then be inferred from the results obtained in quantum mechanics in section 4.10.

Adapting the corresponding expressions, in particular equation (4.59), one obtains a representation of the partition function as a **functional** or **field integral**:

$$\mathcal{Z}(\beta) = \text{tr } \mathbf{U}(\hbar\beta/2, -\hbar\beta/2) = \int [d\varphi(t, x) d\bar{\varphi}(t, x)] \exp[-\mathcal{S}(\bar{\varphi}, \varphi)] \quad (5.11)$$

with the periodic boundary conditions

$$\varphi(\beta/2, x) = \varphi(-\beta/2, x), \quad \bar{\varphi}(\beta/2, x) = \bar{\varphi}(-\beta/2, x).$$

The euclidean action has in general the **non-local** form

$$\begin{aligned} \mathcal{S}(\bar{\varphi}, \varphi) = & - \int_{-\beta/2}^{\beta/2} dt \int d^d x \bar{\varphi}(t, x) \left(\frac{\partial}{\partial t} + \frac{\hbar^2}{2m} \nabla_x^2 + \mu \right) \varphi(t, x) \\ & + \frac{1}{2} \int_{-\beta/2}^{\beta/2} dt \int d^d x d^d y \bar{\varphi}(t, x) \varphi(t, x) V(x - y) \bar{\varphi}(t, y) \varphi(t, y). \end{aligned} \quad (5.12)$$

The addition of a one-particle potential $V_1(x)$ leads simply to the substitution $\mu \mapsto \mu - V_1(x)$.

Again, particle number conservation leads to a $U(1)$ symmetry of the action, corresponding to the transformations

$$\varphi(x) \mapsto e^{i\theta} \varphi(x), \quad \bar{\varphi}(x) \mapsto e^{-i\theta} \bar{\varphi}(x).$$

Remarks.

(i) Let us point out that, depending on the potential, in explicit calculations of field integrals new divergences may appear, which require operations like **regularizations** and **renormalizations**, but these issues will be discussed in the coming lectures.

(ii) We have constructed here a **non-relativistic quantum field theory**. The transition to a relativistic quantum field theory now is essentially a kinematic problem.

5.3.1 The free theory

For free bosons, the action (5.12) reduces to

$$\mathcal{S}(\bar{\varphi}, \varphi) = - \int_{-\beta/2}^{\beta/2} dt d^d x \bar{\varphi}(t, x) \left(\frac{\partial}{\partial t} + \frac{\hbar^2}{2m} \nabla_x^2 + \mu \right) \varphi(t, x),$$

and the field integral is Gaussian.

In a Gaussian theory, all quantities can be expressed in terms of the two-point function. With the convention (5.12), the two-point function

$$\langle \bar{\varphi}(t, x) \varphi(t', x') \rangle_{\text{Gaussian}} \equiv \Delta(t - t', x - x')$$

satisfies the equation

$$\left(\frac{\partial}{\partial t} - \frac{\hbar^2}{2m} \nabla_x^2 - \mu \right) \Delta(t, x) = \delta(t) \delta^{(d)}(x).$$

Setting

$$\Delta(t, x) = \frac{1}{(2\pi\hbar)^d} \int d^d p \, e^{ipx/\hbar} \tilde{\Delta}(t, p),$$

one finds

$$\left(\frac{\partial}{\partial t} + \frac{p^2}{2m} - \mu \right) \tilde{\Delta}(t, p) = \delta(t).$$

The solution of the equation with periodic boundary conditions can be inferred directly from equations (4.36) and (4.35) with $\omega_i \mapsto \omega(p) = p^2/2m - \mu$:

$$\tilde{\Delta}(t, p) = e^{-\omega(p)t} \left[\theta(t) + \frac{1}{e^{\omega(p)\beta} - 1} \right]. \quad (5.13)$$

Due to the periodic boundary conditions in time, the field can be expanded in a Fourier series

$$\varphi(t, x) = \sum_{n=-\infty}^{+\infty} e^{2i\pi nt/\beta} \tilde{\varphi}_n(x), \quad \bar{\varphi}(t, x) = \sum_{n=-\infty}^{+\infty} e^{-2i\pi nt/\beta} \tilde{\bar{\varphi}}_n(x).$$

Then, adapting equation (4.40), one finds

$$\langle \tilde{\bar{\varphi}}_n(p) \tilde{\varphi}_n(-p) \rangle = \frac{1}{\beta(p^2/2m - \mu) - 2i\pi n}. \quad (5.14)$$

5.3.2 The equation of state

The equation of state is obtained by differentiating the partition function (5.11). Assuming a periodic box of linear size L , one finds the density

$$\begin{aligned}\rho(\beta, \mu) &= \frac{1}{\beta L^d} \frac{\partial \ln \mathcal{Z}}{\partial \mu} = \frac{1}{\beta L^d} \int dt d^d x \langle \bar{\varphi}(t, x) \varphi(t, x) \rangle \\ &= \langle \bar{\varphi}(0, 0) \varphi(0, 0) \rangle = \Delta(0, 0),\end{aligned}\quad (5.15)$$

where translation invariance in space and time has been used.

Expressing the result in terms of the Fourier representation (5.13) of the two-point function, one obtains

$$\begin{aligned}\rho(\beta, \mu) &= \frac{1}{(2\pi\hbar)^d} \int d^d p \tilde{\Delta}(0, p) \\ &= \frac{1}{(2\pi\hbar)^d} \int d^d p \left[\theta(0) + \frac{1}{e^{\beta\omega(p)} - 1} \right].\end{aligned}\quad (5.16)$$

This expression coincides with the result (5.5) obtained directly when $\theta(0)$ is chosen to be 0. The algebraically simpler choice $\theta(0) = \frac{1}{2}$ leads to a divergent result, and a term proportional to μ has to be added to the action to remove this additional contribution to ρ .

5.3.3 Zero temperature limit. Real time

In the zero temperature limit, the two-point function (5.13) reduces to

$$\tilde{\Delta}(t, p) = e^{-\omega(p)t} \theta(t).$$

Its Fourier representation in the time variable is

$$\tilde{\Delta}(E, p) = \int dt e^{iEt} \tilde{\Delta}(t, p) = \frac{1}{p^2/2m - \mu - iE}. \quad (5.17)$$

The continuation to real time and, thus, $E \mapsto E e^{-i\theta}$, $0 \leq \theta < \pi/2$, is

$$\tilde{\Delta}(E, p) = \frac{1}{p^2/2m - \mu - E - i\varepsilon}, \quad (5.18)$$

where $\varepsilon \rightarrow 0_+$ indicates how to avoid the pole.

5.3.4 Interactions

When one is interested in large scale phenomena and the interactions are **short range**, the pair potential can be simulated by a Dirac δ -function (but regularized at short distance in dimensions $d > 1$)

$$V(x) = g \delta^d(x), \quad g > 0,$$

and the action becomes **local in space and time**, in the sense that it becomes the integral of a Lagrangian density depending only on the field and its partial derivatives:

$$\begin{aligned} \mathcal{S}(\bar{\varphi}, \varphi) = & \int_{-\beta/2}^{\beta/2} dt d^d x \left[-\bar{\varphi}(t, x) \left(\frac{\partial}{\partial t} + \frac{\hbar^2}{2m} \nabla_x^2 + \mu \right) \varphi(t, x) \right. \\ & \left. + \frac{1}{2} g (\bar{\varphi}(t, x) \varphi(t, x))^2 \right]. \end{aligned} \quad (5.19)$$

5.4 The Helium superfluid transition

The local action (5.19) gives a good model of the He^4 boson system. Moreover, since the superfluid phase transition occurs at low temperature, quantum effects are important. We show now how the formalism that has been presented here, can be indeed been applied to the superfluid transition.

More generally, in presence of **weak repulsive local interactions**, it allows studying the crossover between a **Bose–Einstein condensation** behaviour at shorter distances and, ultimately, a **superfluid transition** at larger distances.

5.4.1 *Leading order or mean field approximation*

The field integral (5.11),

$$\mathcal{Z}(\beta) = \text{tr} \mathbf{U}(\hbar\beta/2, -\hbar\beta/2) = \int [d\varphi(t, x) d\bar{\varphi}(t, x)] \exp[-\mathcal{S}(\bar{\varphi}, \varphi)],$$

in the example of the action (5.19) can be calculated by the steepest descent method.

General arguments indicate that saddle points correspond to constant fields. The saddle point equations, obtained by varying $\bar{\varphi}$ and φ , then read

$$-\mu\varphi + g\varphi^2\bar{\varphi} = 0, \quad -\mu\bar{\varphi} + g\bar{\varphi}^2\varphi = 0.$$

For $\mu < 0$, the equations have only the trivial solution $\varphi = \bar{\varphi} = 0$. The solution is $U(1)$ invariant and the $U(1)$ symmetry is not broken.

In contrast, for $\mu > 0$, they have other solutions: $\bar{\varphi}\varphi = \mu/g$ and one verifies that these are the leading saddle points since the corresponding action in a large volume L^d is

$$\mathcal{S} = -\beta L^d \mu^2 / 2g \Rightarrow \rho = \mu/g.$$

The leading saddle points thus are not $U(1)$ invariant and this corresponds to a **spontaneous breaking of the $U(1)$ symmetry** related to the boson number conservation.

The phase transition, which at leading order, occurs at the value $\mu = 0$ of the chemical potential, describes the **He⁴ superfluid transition**.

However, note that beyond the leading order approximation, the first correction to ρ has, in the thermodynamic limit, the form (5.5)

$$\propto \frac{1}{(2\pi\hbar)^d} \int \frac{d^d p}{e^{\beta(\mathbf{p}^2/2m - \mu)} - 1}$$

and is finite for $\mu = 0$ only for dimensions $d > 2$, as for the Bose–Einstein condensation in a large box.

The marginal dimension $d = 2$ is special and corresponds to a phase transition without symmetry breaking, the peculiar **Kosterlitz–Thouless phase transition**.

5.4.2 The He^4 superfluid transition beyond leading order for $d = 3$

We now specialize to the physical dimension three. Then, the potential is generally parametrized in terms of the s-wave scattering length a (positive because the interaction is assumed repulsive), $g = 4\pi\hbar^2 a/m$. The action becomes

$$\begin{aligned} \mathcal{S}(\bar{\varphi}, \varphi) = & \int_{-\beta/2}^{\beta/2} dt d^3x \left[-\bar{\varphi}(t, x) \left(\frac{\partial}{\partial t} + \frac{\hbar^2}{2m} \nabla_x^2 + \mu \right) \varphi(t, x) \right. \\ & \left. + \frac{1}{2} g (\bar{\varphi}(t, x) \varphi(t, x))^2 \right]. \end{aligned} \quad (5.20)$$

The local potential approximation is justified when the thermal wave length is much larger than the scattering length,

$$\lambda = \hbar \sqrt{2\pi\beta/m} \gg a,$$

that is, at sufficiently low temperature.

In terms of the Fourier components of the field

$$\varphi(t, x) = \sum_{n=-\infty}^{+\infty} e^{2i\pi nt/\beta} \varphi_n(x), \quad \bar{\varphi}(t, x) = \sum_{n=-\infty}^{+\infty} e^{-2i\pi nt/\beta} \bar{\varphi}_n(x),$$

it follows from equation (4.40) that the two-point function reads

$$\langle \tilde{\varphi}_n(p) \tilde{\varphi}_n(-p) \rangle = \frac{1}{\beta(p^2/2m - \mu - iE_n)} \quad \text{with } E_n = 2\pi n/\beta.$$

At the phase transition, $\mu = 0$ at this order, the correlation length $\xi = \hbar/\sqrt{2m\mu}$ diverges. When

$$\xi \gg \lambda$$

the zero mode dominates the large scale behaviour and, thus, one can replace the field, at leading order, by its zero-mode $\varphi_0(x)$. The action reduces to

$$\mathcal{S}(\bar{\varphi}, \varphi) = \beta \int d^3x \left[-\bar{\varphi}_0(x) \left(\frac{\hbar^2}{2m} \nabla_x^2 + \mu \right) \varphi_0(x) + \frac{1}{2} g (\bar{\varphi}_0(x) \varphi_0(x))^2 \right].$$

We recognize the action of a three-dimensional relativistic, euclidean field theory for a complex scalar field. In terms of real components $\boldsymbol{\phi} = (\phi_1, \phi_2)$,

$$\varphi_0(x) = \frac{1}{\hbar} \sqrt{\frac{m}{\beta}} (\phi_1(x) + i\phi_2(x)), \quad \bar{\varphi}_0(x) = \frac{1}{\hbar} \sqrt{\frac{m}{\beta}} (\phi_1(x) - i\phi_2(x)),$$

one recovers the $O(2)$ invariant $(\boldsymbol{\phi}^2)^2$ quantum field theory in a more conventional notation,

$$\mathcal{S}(\boldsymbol{\phi}) = \int d^3x \left[\frac{1}{2} (\nabla_x \boldsymbol{\phi}(x))^2 + \frac{1}{2} r \boldsymbol{\phi}^2(x) + \frac{\tilde{g}}{4!} (\boldsymbol{\phi}^2(x))^2 \right].$$

This theory can then be studied with the standard quantum field theory and renormalization group (RG) methods.

Remark. The non-zero modes can be treated perturbatively and mainly renormalize the parameters of the zero-mode action.

A perturbative calculation of the RG β -function, combined with a Borel-type summation method, shows that the β -function has a non-trivial zero $\tilde{g} = \tilde{g}^* = 26.63 \pm 0.11$, which corresponds to an infra-red fixed point and thus governs the large scale behaviour.

The determination of the fixed point value leads to a first principle calculation of the critical exponents of the superfluid He^4 phase transition: for example, for the correlation exponent ν , low gravity experiments yield $\nu = 0.6708 \pm 0.0004$ while quantum field theory methods and RG lead to $\nu = 0.6703 \pm 0.0015$.

5.5 The Bose gas: time evolution

The formalism discussed in section 4.11 extends to the Bose gas. The evolution operator, in the formalism of second quantization in the presence of a chemical potential μ coupled to the particle number \mathbf{N} , is given by a field integral, generalization of the expression (4.62) to field theory.

One finds

$$\begin{aligned} \langle \varphi'' | \mathbf{U}(t'', t') | \bar{\varphi}' \rangle &= \langle \varphi'' | e^{-i(t''-t)(\mathbf{H}-\mu\mathbf{N})/\hbar} | \bar{\varphi}' \rangle \\ &= \int [d\bar{\varphi}(t, x) d\varphi(t, x)] \exp[i\mathcal{A}(\varphi, \bar{\varphi})/\hbar], \end{aligned} \quad (5.21)$$

where the complex fields $\{\varphi(t, x), \bar{\varphi}(t, x)\}$ satisfy the boundary conditions

$$\bar{\varphi}(t, x') \equiv \bar{\varphi}'(x), \quad \varphi(t, x'') \equiv \varphi''(x).$$

In the example of an external potential $V_1(x)$ and a pair potential $V_2(x-y)$, the action $\mathcal{A}(\varphi, \bar{\varphi})$ is the continuation of the expression (5.12),

$$\begin{aligned} \mathcal{A}(\varphi, \bar{\varphi}) = & -i\hbar\bar{\varphi}(t, x')\varphi(t, x') \\ & + \int dt d^d x \bar{\varphi}(t, x) \left(-i\hbar\frac{\partial}{\partial t} - \frac{\hbar^2}{2m}\nabla_x^2 - V_1(x) + \mu \right) \varphi(t, x) \\ & - \frac{1}{2} \int dt d^d x d^d y \bar{\varphi}(t, x)\varphi(t, x)V_2(x-y)\bar{\varphi}(t, y)\varphi(t, y). \end{aligned}$$

In the absence of an external potential V_1 and for a pseudo-potential $V_2 = G\delta(x-y)$ the action simplifies and becomes local:

$$\begin{aligned} \mathcal{A}(\varphi, \bar{\varphi}) = & -i\hbar\bar{\varphi}(t, x')\varphi(t, x') \\ & + \int dt d^d x \left[\bar{\varphi}(t, x) \left(-i\hbar\frac{\partial}{\partial t} - \frac{\hbar^2}{2m}\nabla_x^2 + \mu \right) \varphi(t, x) \right. \\ & \left. - \frac{1}{2}G(\bar{\varphi}(t, x)\varphi(t, x))^2 \right]. \end{aligned} \tag{5.22}$$

Physical observables can then be calculated, for example, as a series expansion in powers of the interaction, using the propagator (5.18),

$$\tilde{\Delta}(E, p) = \frac{1}{p^2/2m - \mu - E - i\varepsilon}.$$

5.5.1 Classical approximation: Gross–Pitaevski equation

Below, but near the transition temperature of the Bose gas discussed in section 5.1, the field φ is almost **classical** for small coupling.

The field integral (5.21) in the limit $\hbar \rightarrow 0$ can be evaluated by the stationary phase approximation, replacing the field φ by a solution of the equation $\delta\mathcal{A}/\delta\varphi = \delta\mathcal{A}/\delta\bar{\varphi} = 0$. The evolution of the Bose gas is thus approximately described by the classical field (**Gross–Pitaevski**) equation

$$i\hbar\frac{\partial}{\partial t}\varphi(t, x) = \left(-\frac{\hbar^2}{2m}\nabla_x^2 + \mu - G\rho(t, x) \right) \varphi(t, x),$$

where $\rho(t, x)$ is the local condensate density:

$$\rho(t, x) = \bar{\varphi}(t, x)\varphi(t, x),$$

and $\bar{\varphi}$ and φ are complex conjugates. The equation has the form of a **non-linear Schrödinger equation**.

5.6 The relativistic neutral scalar field

Replacing in the non-relativistic action the non-relativistic kinematics by the relativistic kinematics and enforcing **locality**, we construct now a relativistic quantum field theory for a **neutral scalar boson field**.

The classical field $\phi(t, \mathbf{x})$ is real and depends on time t and a $(d - 1)$ -dimensional space coordinate \mathbf{x} . The classical field equations derive from a **Lagrangian density** $\mathcal{L}(\phi)$ of the form (we set the **speed of light** $c = 1$)

$$\mathcal{L}(\phi) = \frac{1}{2} (\dot{\phi}(t, x))^2 - \frac{1}{2} (\nabla_x \phi(t, x))^2 - V(\phi(t, x)), \quad (5.23)$$

where $V(\phi)$ is a polynomial in ϕ .

The Lagrangian density (5.23) has the following properties:

(i) It is **local** in time and space because it depends only on the field $\phi(t, x)$ and its partial derivatives (and not on the product of fields at different points). This property, **locality**, plays a central role in quantum field theory.

(ii) It is invariant under space and time translations since space and time do not appear explicitly in the expression (5.23).

(iii) It is relativistic invariant, that is, invariant under the pseudo-orthogonal group $O(1, d - 1)$ acting linearly on t and \mathbf{x} .

(iv) It leads after quantization (we set $\hbar = 1$), for a suitable class of potentials $V(\phi)$, to a hermitian quantum Hamiltonian bounded from below.

5.6.1 The ϕ^4 field theory

An important example is provided by the so-called ϕ^4 theory where,

$$V(\phi) = \frac{1}{2}m^2\phi^2 + \frac{1}{4!}g\phi^4, \quad g \geq 0.$$

In section 5.12, we argue that this theory has spinless bosons interacting through a pair δ -potential (section 5.3.4) as a non-relativistic limit.

For $g = 0$ (Gaussian or free field theory) the parameter m is the physical mass of the particle associated with the field ϕ . However, for $g \neq 0$, m^2 is generally negative and, thus, this traditional notation is slightly misleading.

5.6.2 Canonical quantization and field integrals

We first quantize the classical theory with the canonical method of quantization. We calculate the Hamiltonian density corresponding to the Lagrangian density (5.23). Lagrangian and Hamiltonian densities are related by Legendre transformation involving $\dot{\phi}$ and $\pi(x)$, conjugate momentum of $\phi(x)$:

$$\mathcal{H}(\pi, \phi) + \mathcal{L}(\dot{\phi}, \phi) - \pi(x)\dot{\phi}(t, x) = 0,$$
$$\pi(x) = \frac{\partial \mathcal{L}}{\partial \dot{\phi}(t, x)} \quad \Leftrightarrow \quad \dot{\phi}(t, x) = \frac{\partial \mathcal{H}}{\partial \pi(x)}.$$

The total Hamiltonian \mathbf{H} is the integral of the Hamiltonian density:

$$\mathbf{H} = \int d^{d-1}x \mathcal{H}[\pi(x), \phi(x)].$$

The coordinates q_i of quantum mechanics are replaced here by the field $\phi(x)$.

The transition between quantum mechanics and quantum field theory can be understood in much the same way as the transition between the discretized action (3.10) and the continuum time limit (3.11).

The quantum Hamiltonian $\hat{\mathbf{H}}$ is obtained by replacing classical fields $\{\pi, \phi\}$ by quantum operators $\{\hat{\pi}, \hat{\phi}\}$ that satisfy the commutation relations (for $\hbar = 1$)

$$[\hat{\phi}(x), \hat{\pi}(x')] = i \delta^{d-1}(x - x'). \quad (5.24)$$

The properties of such a quantum theory can then be studied using the standard methods of operator quantum mechanics. Instead, we now introduce the formalism of field integrals, which generalize the path integrals defined in section 3.3.3 and are closely related to the field integrals introduced in section 5.3.

In the example of the Lagrangian density (5.23), the Hamiltonian density reads

$$\mathcal{H}(\pi, \phi) = \frac{1}{2} \pi^2(x) + \frac{1}{2} [\nabla \phi(x)]^2 + V(\phi(x)). \quad (5.25)$$

The Hamiltonian has an important property: it is quadratic in the momentum $\pi(\mathbf{x})$ and, thus, a generalization of Hamiltonians of the form $p^2/2m + V(q)$. Extending to field theory the ideas presented in section 3.11.2, to ensure unitarity we start from the action written in the Hamiltonian formulation,

$$\mathcal{A}(\pi, \phi) = \int dt d^{d-1}x \left[\pi(t, \mathbf{x}) \dot{\phi}(t, \mathbf{x}) - \mathcal{H}(\pi(t, \mathbf{x}), \phi(t, \mathbf{x})) \right]. \quad (5.26)$$

The matrix elements of the evolution operator $U(t_2, t_1) = e^{-i(t_2-t_1)\mathbf{H}}$ are then given by

$$\langle \phi_2 | U(t_2, t_1) | \phi_1 \rangle = \int [d\phi(t, \mathbf{x}) d\pi(t, \mathbf{x})] \exp [i\mathcal{A}(\pi, \phi)], \quad (5.27)$$

with the boundary conditions $\phi(t_1, \mathbf{x}) = \phi_1(\mathbf{x})$, $\phi(t_2, \mathbf{x}) = \phi_2(\mathbf{x})$.

The action is a quadratic form in π and the Gaussian integration over π can be performed. The result of the integration amounts to replacing π by the solution of the π equation of motion,

$$\frac{\delta \mathcal{A}}{\delta \pi(t, \mathbf{x})} = \dot{\phi}(t, \mathbf{x}) - \pi(t, \mathbf{x}) = 0.$$

This is equivalent to a Legendre transformation and yields the action integral of the Lagrangian density (5.23)

$$\mathcal{A}(\phi) = \int_{t_1}^{t_2} dt \int d^{d-1}x \left\{ \frac{1}{2} \left[(\dot{\phi}(t, \mathbf{x}))^2 - (\nabla_x \phi(t, \mathbf{x}))^2 \right] - V(\phi(t, \mathbf{x})) \right\}. \quad (5.28)$$

The matrix elements of $U(t_2, t_1)$ are then given by the field integral

$$\langle \phi_2 | U(t_2, t_1) | \phi_1 \rangle = \int [d\phi(t, \mathbf{x})] \exp [i\mathcal{A}(\phi)] \quad (5.29)$$

with the boundary conditions $\phi(t_1, \mathbf{x}) = \phi_1(\mathbf{x})$, $\phi(t_2, \mathbf{x}) = \phi_2(\mathbf{x})$.

Note that in a Schrödinger-like formulation of quantum field theory, wave functions are replaced by functionals of classical fields like $\phi_1(x)$ or $\phi_2(x)$ in expression (5.29), which correspond to an infinite number of usual variables.

5.7 The free field

The free field action $\mathcal{A}_0(\phi)$ for the scalar field ϕ is obtained from the general expression (5.28) by specializing to $V(\phi) = m^2\phi^2/2$:

$$\mathcal{A}_0(\phi) = \int dt d^{d-1}x \left[\frac{1}{2}(\dot{\phi}(t, x))^2 - \frac{1}{2}(\nabla_x \phi(t, x))^2 - \frac{1}{2}m^2\phi^2(t, x) \right]. \quad (5.30)$$

We denote by \mathbf{H}_0 the corresponding quantum Hamiltonian.

After continuation to imaginary time $t \mapsto -it$, one obtains the euclidean action

$$\mathcal{S}_0(\phi) = \int_{-\beta/2}^{\beta/2} dt d^{d-1}x \left[\frac{1}{2}(\dot{\phi}(t, x))^2 + \frac{1}{2}(\nabla_x \phi(t, x))^2 + \frac{1}{2}m^2\phi^2(t, x) \right]. \quad (5.31)$$

5.7.1 The euclidean action in Fourier representation

Because the action (5.31) is quadratic in $\phi(t, x)$, the field ϕ can be considered as a collection of harmonic oscillators. We can diagonalize the action by setting

$$\phi(t, x) = \int d^{d-1} \hat{k} e^{i\hat{k}x} \tilde{\phi}(t, \hat{k}).$$

Then,

$$\begin{aligned} \mathcal{S}_0(\phi) = & \frac{1}{2} (2\pi)^{d-1} \int_{-\beta/2}^{\beta/2} dt d^{d-1} \hat{k} [\partial_t \tilde{\phi}(t, \hat{k}) \partial_t \tilde{\phi}(t, -\hat{k}) \\ & + (\hat{k}^2 + m^2) \tilde{\phi}(t, \hat{k}) \tilde{\phi}(t, -\hat{k})]. \end{aligned}$$

The energy splitting for the oscillator corresponding for the momentum \hat{k} is thus

$$\omega(\hat{k}) = \sqrt{\hat{k}^2 + m^2}. \quad (5.32)$$

In the boson interpretation, it is the one-particle energy for a particle of momentum \hat{k} .

The ground state energy. The ground state $|0\rangle$ of the Hamiltonian H_0 is the tensor product of the ground states of the oscillators of momentum \hat{k} . In the particle interpretation it is the empty state, also called the **vacuum**. Then

$$\mathbf{H}_0 |0\rangle = E_0 |0\rangle ,$$

where E_0 is the ground state or vacuum energy. In the usual quantization of the harmonic oscillator it is formally given by the undefined quantity

$$E_0 = \frac{1}{2} \sum_{\hat{k}} \sqrt{m^2 + \hat{k}^2} .$$

To give a precise meaning to E_0 , it is necessary to quantize in a large box of linear size L and to modify the theory at short distance or at large momenta so that the Fourier modes are cut-off at some momentum scale Λ (a space lattice would provide such a cut-off). The Fourier variables \hat{k} are then quantized:

$$\hat{k} = 2\pi\mathbf{n}/L , \quad \mathbf{n} \in \mathbb{Z}^{d-1} .$$

The vacuum energy becomes

$$E_0 = \frac{1}{2} \sum_{\mathbf{n}} \omega(\hat{k}).$$

For L large, sums can be replaced by integrals and $d\mathbf{n} = L^{d-1}/(2\pi)^{d-1} d\hat{k}$. The space volume factorizes, showing as expected that the energy is an extensive, but cut-off dependent quantity:

$$E_0/L^{d-1} = \frac{1}{2} \int^{\Lambda} \frac{d^{d-1}\hat{k}}{(2\pi)^{d-1}} \sqrt{m^2 + \hat{k}^2}. \quad (5.33)$$

The large momentum divergence of the vacuum energy is not important here because in a non-gravitational theory the ground state energy is not an observable: the Hamiltonian can always be shifted by a constant (but **this would no longer be the case if the field theory is coupled to gravitation**).

However, even if the vacuum energy itself is not a physical observable, a variation (imposed for example by a change in boundary conditions) of the vacuum energy may be one (*c.f.*, the **Casimir effect**).

5.7.2 The two-point function

The two-point function, in the infinite volume, **at zero temperature**, is (equation (3.38))

$$\langle \tilde{\phi}(t, \hat{k}) \tilde{\phi}(t, -\hat{k}) \rangle = \frac{1}{(2\pi)^{d-1}} \frac{1}{2\omega(\hat{k})} e^{-\omega(\hat{k})|t|} = \frac{1}{(2\pi)^d} \int d\kappa \frac{e^{i\kappa t}}{\kappa^2 + \hat{k}^2 + m^2}.$$

In the infinite volume, at zero temperature, the euclidean action is $O(d)$ invariant and can be rewritten as

$$\mathcal{S}_0(\phi) = \int d^d x \left[\frac{1}{2} (\nabla_x \phi(t, x))^2 + \frac{1}{2} m^2 \phi^2(t, x) \right]. \quad (5.34)$$

After Fourier transformation over time, one verifies that

$$\langle \phi(t, x) \phi(0, 0) \rangle = \frac{1}{(2\pi)^d} \int d^d k \frac{e^{ikx}}{k^2 + m^2}. \quad (5.35)$$

Field operators. We have shown in section 3.7 that correlation functions have an operator interpretation. In particular, in the zero temperature limit, they are related to the ground state or vacuum expectation value of time-ordered products of operators:

$$\langle \phi(t, x) \phi(0, 0) \rangle = \langle 0 | \hat{\phi}(x) e^{-(H_0 - E_0)|t|} \hat{\phi}(0) | 0 \rangle .$$

The two-point function for real time. To return to real time we perform the inverse rotation $t \rightarrow it$ and simultaneously $\kappa \rightarrow -i\kappa$. We find

$$\langle \phi(t, x) \phi(0, 0) \rangle = \frac{1}{(2\pi)^d} \int dk e^{ikx} \frac{i}{k^2 - m^2 + i\varepsilon} \quad (5.36)$$

with $\varepsilon \rightarrow 0_+$ and $k^2 = \kappa^2 - \hat{k}^2$. The addition of the $i\varepsilon$ contribution directly in the action ensures the convergence of the real time field integral.

5.8 Free field theory and the holomorphic formalism

To further exhibit the relation between relativistic fields and quantum particles, following the example of the non-relativistic field theory of section 4.11, we introduce the **holomorphic formalism**.

We first return again to the free field theory and the action (5.30),

$$\mathcal{A}_0(\phi) = \int dt d^{d-1}x \left[\frac{1}{2} (\dot{\phi}(t, x))^2 - \frac{1}{2} (\nabla_x \phi(t, x))^2 - \frac{1}{2} m^2 \phi^2(t, x) \right].$$

Following the remarks of section 4.7.1, we first write the phase space integral, generalization of the path integral (3.53), and then change variables. The action in the Hamiltonian formalism is

$$\begin{aligned} \mathcal{A}_0(\pi, \phi) = \int dt d^{d-1}x \left\{ \pi(t, x) \dot{\phi}(t, x) - \frac{1}{2} \pi^2(t, x) - \frac{1}{2} [\nabla \phi(t, x)]^2 \right. \\ \left. - \frac{1}{2} m^2 \phi^2(t, x) \right\}. \end{aligned} \tag{5.37}$$

Since the different harmonic oscillators decouple in the momentum basis, we introduce the fields $\varphi(t, \hat{k}), \bar{\varphi}(t, \hat{k})$, analogues of the complex functions $\bar{z}(t), z(t)$ of section 4.11.1 (\hat{k} is the momentum vector).

Using the notation (5.32) $\omega(\hat{k}) = \sqrt{\hat{k}^2 + m^2}$, we define

$$\phi(t, x) = \int \frac{d^{d-1}\hat{k}}{2\omega(\hat{k})} \left[e^{i\hat{k}x} \varphi(t, \hat{k}) + e^{-i\hat{k}x} \bar{\varphi}(t, \hat{k}) \right], \quad (5.38a)$$

$$\pi(t, x) = i \int \frac{d^{d-1}\hat{k}}{2\omega(\hat{k})} \omega(\hat{k}) \left[e^{i\hat{k}x} \varphi(t, \hat{k}) - e^{-i\hat{k}x} \bar{\varphi}(t, \hat{k}) \right]. \quad (5.38b)$$

The sign conventions ensure that when $\bar{\varphi}$ and φ are formally conjugated.

The integration measure $d^{d-1}\hat{k}/2\omega(\hat{k})$ is $O(1, d-1)$ covariant. Indeed, let us introduce the notation (convenient but slightly inconsistent with our euclidean notation) $k = \{k_0, \hat{k}\}$, where k_0 is the energy and \hat{k} the momentum.

Then $k^2 = k_0^2 - \hat{k}^2$ and we define

$$\delta_+(k^2 - m^2) = \delta(k^2 - m^2)\theta(k_0), \quad (5.39)$$

with $\theta(s) = 0$ for $s < 0$, $\theta(s) = 1$ for $s > 0$. One verifies

$$\int \frac{d^{d-1}\hat{k}}{2\omega(\hat{k})} f(\hat{k}) = \int d^d k \delta_+(k^2 - m^2) f(\hat{k}).$$

5.8.1 The action and field integral

In terms of $\varphi, \bar{\varphi}$, the free action (5.37) becomes

$$\mathcal{A}_0(\varphi, \bar{\varphi}) = -(2\pi)^{d-1} \int_{t'}^{t''} dt \frac{d^{d-1}\hat{k}}{2\omega(\hat{k})} \left[i\bar{\varphi}(t, \hat{k})\dot{\varphi}(t, \hat{k}) + \omega(\hat{k})\bar{\varphi}(t, \hat{k})\varphi(t, \hat{k}) \right]. \quad (5.40)$$

The formalism again confirms (see also sections 4.11, 4.11.1) that one particle states are relativistic particles of momentum \hat{k} and energy $\omega(\hat{k})$. However, a drawback is that the holomorphic formalism is not explicitly local.

Field integral. A representation of the free evolution operator U_0 as a field integral in the holomorphic formalism follows

$$U_0(t'', t'; \varphi'', \bar{\varphi}') = \int [\omega^{-1}(\hat{k}) d\varphi(t, \hat{k}) d\bar{\varphi}(t, \hat{k})] \exp [i\mathcal{A}_0(\varphi, \bar{\varphi})],$$

where $\mathcal{A}_0(\varphi, \bar{\varphi})$ is the action (5.40).

Interactions. Locality implies that the interaction terms must be local polynomials of the field and derivatives. The decomposition (5.38a) then immediately shows that interaction terms like ϕ^4 will involve contributions that **do not conserve the number of particles**.

5.8.2 Fock's space

In the holomorphic formalism, the differences with the non-relativistic example discussed in section 4.11 are mostly of kinematic nature.

For completeness, we briefly review the construction of the corresponding Fock's space. We work in the momentum representation, where the Hamiltonian is diagonal.

Let $\psi_1(\hat{k}), \psi_2(\hat{k})$ be two wave functions associated with one-particle states of a boson of mass m . The scalar product of two states $|\psi_1\rangle, |\psi_2\rangle$ can be written in the relativistic covariant form

$$\langle \psi_1 | \psi_2 \rangle = (2\pi)^{d-1} \int \frac{d^{d-1}\hat{k}}{2\omega(\hat{k})} \psi_1^*(\hat{k}) \psi_2(\hat{k}).$$

We now introduce a complex field $\varphi(\hat{k})$ and the generating functional $\Psi(\varphi)$ of general n -particle wave functions for bosons

$$\Psi(\varphi) = \sum_{n=0}^{\infty} \frac{(2\pi)^{n(d-1)}}{n!} \int \psi(\hat{k}_1, \hat{k}_2, \dots, \hat{k}_n) \prod_{i=1}^n \varphi(\hat{k}_i) \frac{d^{d-1}\hat{k}_i}{2\omega(\hat{k}_i)},$$

where $\psi(\hat{k}_1, \hat{k}_2, \dots, \hat{k}_n)$ is a wave function totally symmetric in the momenta \hat{k}_i . The direct sum of the n -particle spaces for all n is called **Fock space**.

The scalar product of two vectors Ψ_1 and Ψ_2 in Fock's space takes the form

$$\begin{aligned} \langle \Psi_2 | \Psi_1 \rangle &= \int [\omega^{-1}(\hat{k}) d\varphi(\hat{k}) d\bar{\varphi}(\hat{k})] \\ &\times \exp \left[-(2\pi)^{d-1} \int \frac{d^{d-1}\hat{k}}{2\omega(\hat{k})} \bar{\varphi}(\hat{k}) \varphi(\hat{k}) \right] \overline{\Psi_2(\varphi)} \Psi_1(\varphi). \end{aligned} \quad (5.41)$$

5.8.3 Operators in Fock's space

The free action (5.40) shows that the one-particle Hamiltonian has an energy spectrum of the form $\omega(\hat{k})$. Acting on $\Psi(\varphi)$, the free Hamiltonian is thus represented by the operator

$$\mathbf{H}_0 = \int d^{d-1}\hat{k} \varphi(\hat{k}) \omega(\hat{k}) \frac{\delta}{\delta \varphi(\hat{k})} + E_0,$$

where E_0 is the ground state or vacuum, that is, the zero-particle state energy.

The kernel representing the identity which corresponds to the scalar product (5.41) is

$$\mathcal{I}(\varphi, \bar{\varphi}) = \exp \left[(2\pi)^{d-1} \int \frac{d^{d-1} \hat{k}}{2\omega(\hat{k})} \bar{\varphi}(\hat{k}) \varphi(\hat{k}) \right]. \quad (5.42)$$

The kernel associated with the Hamiltonian follows

$$\mathbf{H}_0 \mapsto \left[\frac{1}{2} (2\pi)^{d-1} \int d^{d-1} \hat{k} \bar{\varphi}(\hat{k}) \varphi(\hat{k}) \right] \mathcal{I}(\varphi, \bar{\varphi}).$$

Note that the free Hamiltonian commutes with the particle number operator \mathbf{N} :

$$\mathbf{N} = \int d^{d-1} \hat{k} \varphi(\hat{k}) \frac{\delta}{\delta \varphi(\hat{k})} \mapsto (2\pi)^{d-1} \int \frac{d^{d-1} \hat{k}}{2\omega(\hat{k})} \varphi(\hat{k}) \bar{\varphi}(\hat{k}) \mathcal{I}(\varphi, \bar{\varphi})$$

and thus $[\mathbf{N}, \mathbf{H}_0] = 0$, a property that, in general, no longer holds in the presence of **local** interactions.

5.8.4 Two-point function

The ϕ -field two-point function, expressed as the expectation value of a time-ordered product of two fields (see for example section 3.7, equation (3.30)), is given by

$$\begin{aligned} \langle 0 | \mathbf{T}[\tilde{\phi}(t, \hat{k}) \tilde{\phi}(\hat{0}, \hat{k}')] | 0 \rangle &= \langle 0 | \tilde{\phi}(\hat{k}) e^{-i(\mathbf{H}_0 - E_0)|t|} \tilde{\phi}(\hat{k}') | 0 \rangle \\ &= (2\pi)^{1-d} \frac{1}{2\omega(\hat{k})} \delta^{d-1}(\hat{k} + \hat{k}') e^{-i\omega(\hat{k})|t|}. \end{aligned} \quad (5.43)$$

After Fourier transformation over time, one recovers a form of expression (5.36),

$$\frac{1}{2\pi} \int e^{ik_0 t} dt \langle 0 | \mathbf{T}[\tilde{\phi}(t, \hat{k}) \tilde{\phi}(0, \hat{k}')] | 0 \rangle = \frac{1}{(2\pi)^d} \delta^{d-1}(\hat{k} + \hat{k}') \frac{i}{k_0^2 - \omega^2(\hat{k}) + i\varepsilon}, \quad (5.44)$$

($k_0^2 - \omega^2(\hat{k}) = k^2 - m^2$) where the $i\varepsilon$ term in the denominator indicates that we have to add a small positive imaginary part.

The real time two-point function is a distribution in the mathematical sense, boundary value of an analytic function

$$\frac{i}{k_0^2 - \omega^2(\hat{k}) + i\varepsilon} \equiv 2\pi\delta(k_0^2 - \omega^2(\hat{k})) + i\text{PP}\frac{1}{k_0^2 - \omega^2(\hat{k})},$$

where **PP** means principal part.

5.9 The S -matrix: generalities

Having explored the relation between fields and particles, we can now define the scattering S -matrix. We first calculate explicitly the scattering by an external source. The result will lead to a perturbative expression for the S -matrix in a general interacting theory.

5.9.1 Scattering by an external source

To the free action (5.30),

$$\mathcal{A}_0(\phi) = \int dt d^{d-1}x \left[\frac{1}{2} (\dot{\phi}(t, x))^2 - \frac{1}{2} (\nabla_x \phi(t, x))^2 - \frac{1}{2} m^2 \phi^2(t, x) \right],$$

we add a source term, corresponding to the linear coupling of the field ϕ to an external classical source $J(t, x)$. The resulting action \mathcal{A}_G then takes the form

$$\mathcal{A}_G(\phi) = \mathcal{A}_0(\phi) + \int dt d^{d-1}x J(t, x) \phi(t, x).$$

We introduce the complex fields $\varphi, \bar{\varphi}$ (equation (5.38a)) and the Fourier components of the source,

$$J(t, x) = \int e^{i\hat{k}x} \tilde{J}(t, \hat{k}) d\hat{k}.$$

The action \mathcal{A}_G then reads

$$\mathcal{A}_G(\varphi, \bar{\varphi}) = \mathcal{A}_0(\varphi, \bar{\varphi}) + (2\pi)^{d-1} \int dt \frac{d\hat{k}}{2\omega(\hat{k})} \left[\tilde{J}(t, -\hat{k})\varphi(t, \hat{k}) + \tilde{J}(t, \hat{k})\bar{\varphi}(t, \hat{k}) \right],$$

where $\mathcal{A}_0(\varphi, \bar{\varphi})$ is the action (5.40):

$$\mathcal{A}_0(\varphi, \bar{\varphi}) = -(2\pi)^{d-1} \int_{t'}^{t''} dt \frac{d^{d-1}\hat{k}}{2\omega(\hat{k})} \left[i\bar{\varphi}(t, \hat{k})\dot{\varphi}(t, \hat{k}) + \omega(\hat{k})\bar{\varphi}(t, \hat{k})\varphi(t, \hat{k}) \right].$$

A straightforward adaptation of the expression (4.64) yields the holomorphic S -matrix:

$$\begin{aligned} \ln S_G(J, \varphi, \bar{\varphi}) &= (2\pi)^{d-1} \int \frac{d\hat{k}}{2\omega(\hat{k})} K(\hat{k}) \quad \text{with} \\ K(\hat{k}) &= \varphi(\hat{k})\bar{\varphi}(\hat{k}) + i \int dt \left[\varphi(\hat{k}) e^{i\omega(\hat{k})t} \tilde{J}(t, -\hat{k}) + \bar{\varphi}(\hat{k}) e^{-i\omega(\hat{k})t} \tilde{J}(t, \hat{k}) \right] \\ &\quad - \frac{1}{2} \int dt_1 dt_2 \tilde{J}(t_1, -\hat{k}) e^{-i\omega(\hat{k})|t_2-t_1|} \tilde{J}(t_2, \hat{k}). \end{aligned}$$

(In the last term we have symmetrized in $\hat{k} \mapsto -\hat{k}$ and then $t_1 \leftrightarrow t_2$.)

As explained in section 4.11.1, the coefficients of the scattering matrix are obtained by expanding the functional in powers of φ and $\bar{\varphi}$.

Introducing the time Fourier components

$$\tilde{J}(t, \hat{k}) = \int dk_0 e^{-ik_0 t} \tilde{J}(k_0, \hat{k}),$$

one obtains the more useful expression

$$\begin{aligned} \ln S_G(J, \varphi, \bar{\varphi}) &= (2\pi)^{d-1} \int \frac{d\hat{k}}{2\omega_{\hat{k}}} \varphi(\hat{k}) \bar{\varphi}(\hat{k}) + i(2\pi)^d \int d\hat{k} dk_0 \tilde{J}(k_0, \hat{k}) \\ &\times \left[\delta_+(k_0^2 - \hat{k}^2 - m^2) \varphi(-\hat{k}) + \delta_-(k_0^2 - \hat{k}^2 - m^2) \bar{\varphi}(\hat{k}) \right] \\ &- \frac{1}{2} (2\pi)^d \int d\hat{k} dk_0 \tilde{J}(-k_0, \hat{k}) \frac{i}{k_0^2 - \hat{k}^2 - m^2 + i\varepsilon} \tilde{J}(k_0, \hat{k}) \end{aligned} \quad (5.45)$$

with the notation (see definition (5.39))

$$\delta_{\pm}(k_0^2 - \hat{k}^2 - m^2) = \theta(\pm k_0) \delta(k_0^2 - \hat{k}^2 - m^2).$$

In the coefficient of the term quadratic in J we recognize the free two-point function (5.44).

5.9.2 General interacting theory

An interaction term $V_I(\phi)$ can then be added to the free action,

$$\mathcal{A}(\phi) = \int dt d^{d-1}x \left\{ \frac{1}{2} \left[(\dot{\phi}(t, x))^2 - (\nabla_x \phi(t, x))^2 - m^2 \phi^2(t, x) \right] - V_I(\phi(t, x)) \right\}, \quad (5.46)$$

where ϕ has to be expressed in terms of $\varphi, \bar{\varphi}$. Using the definition of the functional differentiation applied on the field integral, one can derive the form of the S -matrix for the interacting theory

$$S(\varphi, \bar{\varphi}) = \exp \left[-i \int dt d^{d-1}x V_I \left(\frac{1}{i} \frac{\delta}{\delta J} \right) \right] S_G(J, \varphi, \bar{\varphi}) \Big|_{J=0}. \quad (5.47)$$

The S -matrix thus has a Feynman diagram expansion with internal propagators Δ given by the quadratic term in J in expression (5.45):

$$\Delta(k_0, \hat{k}) = \frac{i}{k_0^2 - \hat{k}^2 - m^2 + i\varepsilon} \equiv \frac{i}{k^2 - m^2 + i\varepsilon}. \quad (5.48)$$

We note that we have indeed obtained a propagator, which otherwise would be singular on the mass-shell $k^2 = k_0^2 - \hat{k}^2 = m^2$, with the usual $i\varepsilon$ prescription.

Unitarity. With our conventions the unitarity of the S -matrix takes the functional form

$$\begin{aligned} & \int [d\bar{\varphi}'(\hat{k})d\varphi'(\hat{k})] S^*(\varphi', \bar{\varphi}) \mathcal{S}(\varphi', \bar{\varphi}) \exp \left[-(2\pi)^{d-1} \int \frac{d\hat{k}}{2\omega(\hat{k})} \varphi'(\hat{k}) \bar{\varphi}'(\hat{k}) \right] \\ & = \exp \left[(2\pi)^{d-1} \int \frac{d\hat{k}}{2\omega(\hat{k})} \varphi(\hat{k}) \bar{\varphi}(\hat{k}) \right]. \end{aligned}$$

Discussion. We have constructed our basis of states from the eigenstates of the unperturbed Hamiltonian. More generally, we can take another harmonic oscillator basis corresponding to a different mass, at the price of adding to the interaction terms quadratic in the field.

Actually, and this will become clearer when we discuss the structure of the ground state in field theory, if we take an arbitrary basis, in general, all eigenstates of the interacting Hamiltonian will be orthogonal to all vectors of the basis, **a property specific to systems with an infinite number of degrees of freedom.**

Moreover, the Hamiltonian of a massive theory has a unique, translation invariant, lowest energy excited state (in the case of several fields this can be generalized to all super-selection sectors). The physical mass m (or inverse correlation length in the statistical language) is defined as the energy of this state. This defines the **zero momentum one-particle state.**

A more general one-particle state is obtained by boosting the zero momentum state, that is, performing a $O(1, d - 1)$ transformation, and creating a one-particle state of momentum \hat{k} and energy $\omega(\hat{k})$. Additional eigenstates have energies at least equal to $2m$.

Therefore, we have to take as vacuum state **the true ground state of the full Hamiltonian**, and as asymptotic free states, free particles with the true physical mass. These conditions implicitly define a reference free theory with action \mathcal{A}_0 , and ensures that it describes the asymptotic states at large times.

The vacuum state and the physical mass can be calculated in perturbation theory. To calculate scattering amplitudes one has to perform order by order **field and mass renormalizations**, which involves, in particular, taking the physical mass as a parameter of the perturbative expansion by inverting the relation between the physical mass as defined by the pole of the two-point function and the coefficient of ϕ^2 as it appears in the action.

Finally, note that the functional integral has to be normalized by the condition $S(0,0) = 1$, which means that we divide by a factor related to difference in energies between the true and the unperturbed ground state.

5.10 S -matrix and field asymptotic conditions

Since the action is only local when written in terms of the initial real field ϕ , it is convenient to find an expression of the S -matrix in the ϕ formalism.

We know how to calculate the matrix elements of the evolution operator by integrating over the field ϕ .

We now compare this expression of the evolution operator with the explicit form (5.47) of the S -matrix as derived from the holomorphic representation.

5.10.1 *The Gaussian integral in an external source and S -matrix*

We first consider the Gaussian theory in an external source

$$\mathcal{Z}_G(J) = \int [d\phi] \exp \left[i\mathcal{A}_0(\phi) + i \int dt d^{d-1}x J(t, x)\phi(t, x) \right]. \quad (5.49)$$

The action can be written in terms of the Fourier components of the source J and the field ϕ ,

$$\phi(t, x) = \int dk e^{i\hat{k}x - ik_0t} \tilde{\phi}(k_0, \hat{k}).$$

The total action becomes

$$\begin{aligned} \mathcal{A}(\phi) = (2\pi)^d \int dk_0 d\hat{k} & \left[\frac{1}{2} \tilde{\phi}(-k_0, -\hat{k}) (k_0^2 - \hat{k}^2 - m^2) \tilde{\phi}(k_0, \hat{k}) \right. \\ & \left. + J(-k_0, -\hat{k}) \tilde{\phi}(k_0, \hat{k}) \right]. \end{aligned} \quad (5.50)$$

Unlike the euclidean functional integral, the functional integral for the evolution operator has convergence problems because classical field equations have non-trivial solutions. This problem has already been discussed in section 4.11.2, and we use the same strategy here.

We define the functional integral as the analytic continuation in time of the euclidean path integral. We perform a rotation in the time complex plane $t \mapsto te^{i\theta}$ where θ varies between 0 (the euclidean theory) and $\pi/2$, (the Minkowsky theory). In the energy variable k_0 the corresponding rotation is $k_0 \mapsto k_0 e^{-i\theta}$.

As we have indicated this amounts to adding to m^2 an infinitesimal negative imaginary part which ensures the convergence of the field integral (5.49) for large fields. The generating functional $\mathcal{Z}_G(J)$ can then be calculated and one finds

$$\ln \mathcal{Z}_G(J) = -\frac{1}{2}(2\pi)^d \int dk_0 d\hat{k} J(k_0, \hat{k}) \Delta(k_0, \hat{k}) J(-k_0, -\hat{k}), \quad (5.51)$$

where $\Delta(k_0, \hat{k})$ is the free propagator

$$\Delta(k_0, \hat{k}) = \frac{i}{k_0^2 - \hat{k}^2 - m^2 + i\varepsilon} \equiv \frac{i}{k^2 - m^2 + i\varepsilon}. \quad (5.52)$$

We note that the propagator obtained by this prescription is identical to the internal propagator (5.48) that appears in the Feynman graph expansion of the S -matrix. The analytic continuation leads to an $i\varepsilon$ rule for real time Feynman diagrams.

S-matrix in an external source. Comparing the expressions (5.51) and (5.45), we see that the quadratic term is reproduced but not the term linear in the source. This term corresponds to an addition to the field $\tilde{\phi}$:

$$\tilde{\phi}(k_0, \hat{k}) \mapsto \tilde{\phi}(k_0, \hat{k}) + \tilde{\phi}_0(k_0, \hat{k})$$

with

$$\tilde{\phi}_0(k_0, \hat{k}) = \delta(k_0^2 - \hat{k}^2 - m^2) \left[\varphi(\hat{k})\theta(-k_0) + \bar{\varphi}(-\hat{k})\theta(k_0) \right]. \quad (5.53)$$

The additional term $\tilde{\phi}_0(k_0, \hat{k})$ thus is, in some specific parametrization, the general solution of the free classical field equation

$$(k_0^2 - \hat{k}^2 - m^2)\tilde{\phi}_0(k_0, \hat{k}) = 0.$$

It is non-vanishing only on the mass hyperboloid $k^2 = m^2$. The parametrization (5.53) of the solution reflects the property that the mass hyperboloid has two disconnected components, depending on the sign of the energy k_0 .

As we have noted in section 4.11.2, we can shift the field ϕ taking $\phi + \phi_0$ as the integration variable. The shifted field ϕ then satisfies scattering boundary conditions and the S -matrix can thus be derived from the functional integral

$$\mathcal{Z}_G(J) = \int [d\phi] \exp \left[i\mathcal{A}_0(\phi) - i\mathcal{A}_0(\phi_0) + i \int dt dx J(t, x)\phi(t, x) \right]. \quad (5.54)$$

The interpretation is the following: the field ϕ in the functional integral (5.49) satisfies general free field boundary conditions, $\phi \rightarrow \phi_0$, and its two-point function or propagator is then given by equation (5.52).

General interaction. The general functional representation (5.47) can then be rewritten in a different way. Introducing the form (5.54) of \mathcal{Z}_G in (5.47) and applying the functional derivatives, one finds

$$\mathcal{S}(\varphi, \bar{\varphi}) = \mathcal{I}(\varphi, \bar{\varphi}) \int [d\phi] \exp i [\mathcal{A}(\phi) - \mathcal{A}_0(\phi_0)], \quad (5.55)$$

where \mathcal{I} is the identity kernel (5.42), and the field ϕ satisfies fixed free field asymptotic boundary conditions.

The expression (5.55), up to the factor \mathcal{I} , is a functional integral in the presence of a background field ϕ_0 . This field integral differs from the vacuum amplitude only in the boundary conditions, which are free field boundary conditions.

This result is consistent with the analysis of section 3.12.1. We have shown that in quantum mechanics S -matrix elements can be calculated from the path integral representation of the evolution operator, by integrating over paths which satisfy prescribed classical scattering boundary conditions, that is, which correspond to asymptotic free classical motion.

In particular, the starting point of the semi-classical expansion is a classical scattering trajectory. The arguments can be generalized to quantum field theory with massive particles (to ensure proper cluster properties and thus the existence of an S -matrix).

Remark. Considerations based on asymptotic field boundary conditions, or the more direct considerations of section 5.8 lead to the same perturbative S -matrix.

However, as suggested by the discussion given at the beginning of section 3.12.1, the preceding considerations generalize to the scattering of **solitons**, that is, states obtained by expanding the functional integral around **finite energy static solutions of the complete classical field equations**

$$\frac{\delta \mathcal{A}(\phi)}{\delta \phi(x)} = 0.$$

In this case, the S -matrix of soliton scattering is obtained by expanding the field integral around classical soliton scattering solutions of the complete field equations.

5.10.2 S -matrix and correlation functions

Alternatively, let us consider the following expression for a general interaction,

$$\mathcal{Z}(\mathcal{J}) = \exp \left[-i \int d^d x V_I \left(\frac{1}{i} \frac{\delta}{\delta J(x)} \right) \right] \exp \left[-\frac{1}{2} (\mathcal{J} + J) \Delta (\mathcal{J} + J) \right] \Big|_{J=0}, \quad (5.56)$$

where \mathcal{J} is an additional external source and the last term a formal representation of

$$\begin{aligned} & \frac{1}{2} (\mathcal{J} + J) \Delta (\mathcal{J} + J) \\ & \equiv \frac{1}{2} (2\pi)^d \int d^d k (\tilde{J}(-k) + \tilde{\mathcal{J}}(-k)) \frac{i}{k^2 - m^2 + i\varepsilon} (\tilde{J}(k) + \tilde{\mathcal{J}}(k)). \quad (5.57) \end{aligned}$$

Comparing expression (5.56) with expression (5.45),

$$\begin{aligned} \ln S_G(J, \varphi, \bar{\varphi}) &= (2\pi)^{d-1} \int \frac{d\hat{k}}{2\omega_{\hat{k}}} \varphi(\hat{k}) \bar{\varphi}(\hat{k}) \\ &+ i(2\pi)^d \int dk \tilde{J}(k) \left[\delta_+(k^2 - m^2) \varphi(-\hat{k}) + \delta_-(k^2 - m^2) \bar{\varphi}(\hat{k}) \right] \\ &- \frac{1}{2} (2\pi)^d \int dk \tilde{J}(-k) \frac{i}{k^2 - m^2 + i\varepsilon} \tilde{J}(k), \end{aligned}$$

combined with equation (5.47),

$$S(\varphi, \bar{\varphi}) = \exp \left[-i \int dt dx V_I \left(\frac{1}{i} \frac{\delta}{\delta J} \right) \right] S_G(J, \varphi, \bar{\varphi}) \Big|_{J=0},$$

we see that the two expressions are very close if one sets

$$\frac{i}{k^2 - m^2 + i\varepsilon} \tilde{J}(k_0, \hat{k}) \mapsto -i\delta(k^2 - m^2) \left[\varphi(\hat{k})\theta(-k_0) + \bar{\varphi}(-\hat{k})\theta(k_0) \right]. \quad (5.58)$$

Therefore, we conclude that S -matrix elements can be obtained from real time correlation functions by first multiplying them by the product of external inverse propagators, and then by restricting the external momenta to the mass-shell $k^2 = m^2$.

This does not imply that the result vanishes. Indeed, correlation functions have poles on the mass-shell. The final answer is proportional to the so-called **amputated correlation functions** on mass-shell.

Connected contributions. The relation between correlation functions and S -matrix elements shows that the matrix elements as defined here have disconnected contributions. Instead, the new functional

$$\mathcal{T}(\varphi, \bar{\varphi}) = i \ln S(\varphi, \bar{\varphi}), \quad (5.59)$$

is the generating functional of connected scattering amplitudes (see section 6.10.1).

Crossing symmetry. We see that only a linear combination of φ and $\bar{\varphi}$ appears, with identical coefficients, up to the sign of the energy. The sign of k_0 specifies the incoming and outgoing particles. This has deep implications, specific to relativistic quantum field theory: in $d > 2$ dimensions, the same analytic functions lead to scattering amplitudes of different physical processes, a property known as crossing symmetry.

5.10.3 The ϕ^3 example

We illustrate the analysis by calculating a four-point scattering amplitude in the simple ϕ^3 field theory, in the tree approximation. We consider the action

$$\mathcal{A}(\phi) = \int dt d^{d-1}x \left[\frac{1}{2} (\dot{\phi}(t, x))^2 - \frac{1}{2} (\nabla_x \phi(t, x))^2 - \frac{1}{2} m^2 \phi^2(t, x) - \frac{1}{3!} g \phi^3(t, x) \right].$$

We introduce the Fourier components of the field ϕ ,

$$\phi(t, x) = \int e^{-ik_0 t + i\hat{k}x} \tilde{\phi}(k) d^d k.$$

In terms of Fourier components, the field equation takes the form

$$(k^2 - m^2) \tilde{\phi}(k) - \frac{1}{2} g \int d^d q \tilde{\phi}(q) \tilde{\phi}(k - q) = 0. \quad (5.60)$$

The equation can be solved as a series in the coupling constant g starting from the solution (5.53) of the free equation:

$$\tilde{\phi}_0(k) = \delta(k^2 - m^2) \left[\varphi(\hat{k})\theta(-k_0) + \bar{\varphi}(-\hat{k})\theta(k_0) \right].$$

The classical solution at order g is

$$\tilde{\phi}(k) = \tilde{\phi}_0(k) + \frac{g}{2(k^2 - m^2)} \int d^d q \tilde{\phi}_0(q)\tilde{\phi}_0(k - q) + O(g^2).$$

By looking for perturbative solutions of the field equation we have explicitly excluded scattering states corresponding to bound states or solitons (see the remark at the end of section 5.10.1).

Using equation (5.60) we can rewrite \mathcal{T} in the tree approximation as

$$\begin{aligned} \mathcal{T}(\phi_0) &= i \ln S(\phi_0) \\ &= -\frac{1}{12}g(2\pi)^d \int d^d k_1 d^d k_2 d^d k_3 \delta^{(d)}(k_1 + k_2 + k_3) \tilde{\phi}(k_1)\tilde{\phi}(k_2)\tilde{\phi}(k_3). \end{aligned}$$

We then replace ϕ by its expansion in powers of g . The term of order g , which would describe one ϕ particle decaying into two, vanishes by energy conservation. The next term of order g^2 has the form

$$-\frac{1}{8}g^2(2\pi)^d \int \delta^{(d)}(k_1 + k_2 + k_3 + k_4) \frac{1}{(k_1 + k_2)^2 - m^2} \prod_{i=1}^4 dk_i \tilde{\phi}_0(k_i).$$

The connected four-particle scattering amplitude is then obtained by differentiating with respect to $\tilde{\phi}_0(k)$. The result is the product of a factor that contains the momentum conservation,

$$(2\pi)^d \delta^{(d)}(k_1 + k_2 + k_3 + k_4),$$

and an amplitude ($k_i^2 = m^2$),

$$-\frac{g^2}{(k_1 + k_2)^2 - m^2} - \frac{g^2}{(k_1 + k_3)^2 - m^2} - \frac{g^2}{(k_1 + k_4)^2 - m^2}.$$

The term we have calculated also contains, in principle, the decay of one particle into three but again this process vanishes by energy conservation.

Higher orders in g yield five, six ... particle scattering amplitudes.

5.11 Two-point function: spectral representation and field renormalization

We now derive the spectral representation of the two-point function and its implication on field renormalization. This can more conveniently be done in the **euclidean formulation**.

We define the field operator in the **Schrödinger representation** $\hat{\phi}(x)$ in such a way that $\langle 0|\hat{\phi}|0\rangle = 0$, where $|0\rangle$ is the ground state or vacuum. This can always be achieved by a constant shift. It follows from the discussion of section 3.7 (equation (3.31)) that the two-point function is given by

$$W^{(2)}(x - y; t - u) = \langle 0| \hat{\phi}(x) e^{-(\mathbf{H} - E_0)|t - u|} \hat{\phi}(y) |0\rangle,$$

where E_0 is the ground state or vacuum energy.

5.11.1 Spectral representation

Symbolically, we denote by $|\alpha\rangle$ a complete set of eigenvectors of the Hamiltonian and we denote by $E_0 + \varepsilon_\alpha$ the corresponding energy eigenvalues. Then,

$$e^{-(\mathbf{H}-E_0)|t|} = \int d\alpha |\alpha\rangle e^{-\varepsilon_\alpha|t|} \langle\alpha|$$

and, thus,

$$W^{(2)}(x - y; t) = \int d\alpha \langle 0 | \hat{\phi}(x) | \alpha \rangle e^{-\varepsilon_\alpha|t|} \langle \alpha | \hat{\phi}(y) | 0 \rangle.$$

We define the Fourier transform of the field operator by

$$\hat{\phi}(\hat{k}) = \frac{1}{(2\pi)^{d-1}} \int d^{d-1}x e^{-i\hat{k}x} \hat{\phi}(x).$$

We then calculate the two-point correlation function $W^{(2)}$ in the Fourier representation. From translation invariance, we know that the Fourier transform has the form

$$\begin{aligned} \delta^{d-1}(\hat{k} + \hat{k}') \tilde{W}^{(2)}(t, \hat{k}) &= (2\pi)^{d-1} \langle 0 | \hat{\phi}(\hat{k}) e^{-|t|(\mathbf{H}-E_0)} \hat{\phi}(\hat{k}') | 0 \rangle, \\ &= (2\pi)^{d-1} \int d\alpha \langle 0 | \hat{\phi}(\hat{k}) | \alpha \rangle e^{-\varepsilon_\alpha |t|} \langle \alpha | \hat{\phi}(\hat{k}') | 0 \rangle. \end{aligned} \quad (5.61)$$

The right hand side is a distribution with a support reduced to $\hat{k}' = -\hat{k}$. In this limit, since $\hat{\phi}(-\hat{k}) = \hat{\phi}^\dagger(\hat{k})$, the left hand side is a sum of positive terms. (A more careful argument would involve a finite box with quantized momenta.)

We thus find

$$\tilde{W}^{(2)}(t, \hat{k}) = \int d\alpha \rho(\alpha, \hat{k}) e^{-|t|\varepsilon_\alpha},$$

where ρ is a positive measure.

The Fourier transform with respect to time is given by

$$\begin{aligned}\tilde{W}^{(2)}(k_0, \hat{k}) &= \int dt e^{-ik_0 t} \int d\alpha \rho(\alpha, \hat{k}) e^{-|t|\varepsilon(\alpha)} \\ &= \int d\alpha \frac{2\varepsilon(\alpha)\rho(\alpha, \hat{k})}{k_0^2 + \varepsilon^2(\alpha)}.\end{aligned}$$

The relativistic $O(d)$ invariance allows to set $\hat{k} = 0$ and replace k_0^2 by k^2 without changing the right hand side. We conclude

$$\tilde{W}^{(2)}(k) = \int d\alpha \frac{\rho(\alpha)}{k^2 + \alpha^2} \tag{5.62}$$

with $\rho(\alpha) = 2\varepsilon(\alpha)\rho(\alpha, 0)$ is a positive measure. This form is called the Källén–Lehmann (KL) representation.

5.11.2 Field renormalization

Conversely, the Fourier transform with respect to the k_0 now is

$$\begin{aligned} W^{(2)}(t, \hat{k}) &= \frac{1}{2\pi} \int dk_0 e^{ik_0 t} \tilde{W}^{(2)}(k) = \frac{1}{2\pi} \int dk_0 e^{ik_0 t} \int d\alpha \frac{\rho(\alpha)}{k^2 + \alpha^2} \\ &= \int d\alpha \frac{\rho(\alpha)}{2\sqrt{\hat{k}^2 + \alpha^2}} e^{-|t|\sqrt{\hat{k}^2 + \alpha^2}}. \end{aligned} \quad (5.63)$$

For $t > 0$, taking the derivative with respect to time and the limit $t = 0$, one concludes

$$\left. \frac{\partial}{\partial t} W^{(2)}(\hat{k}, t) \right|_{t \rightarrow 0_+} = -\frac{1}{2} \int d\alpha \rho(\alpha). \quad (5.64)$$

Returning to the definition (5.61), taking for $t > 0$ the derivative with respect to time and the limit $t = 0$, one finds

$$\delta^{d-1}(\hat{k} + \hat{k}') \left. \frac{\partial}{\partial t} W^{(2)}(\hat{k}, t) \right|_{t \rightarrow 0_+} = -(2\pi)^{d-1} \langle 0 | \hat{\phi}(\hat{k})(\mathbf{H} - E_0)\hat{\phi}(\hat{k}') | 0 \rangle. \quad (5.65)$$

The product $(\mathbf{H} - E_0)\hat{\phi}$ in the right hand side can be replaced by the commutator $[\mathbf{H}, \hat{\phi}]$. Indeed,

$$\langle 0 | \hat{\phi}[\mathbf{H}, \hat{\phi}] | 0 \rangle = \langle 0 | \hat{\phi} (\mathbf{H}\hat{\phi} | 0 \rangle - \hat{\phi}\mathbf{H} | 0 \rangle) = \langle 0 | \hat{\phi}(\mathbf{H} - E_0)\hat{\phi} | 0 \rangle.$$

Similarly, on the left hand side,

$$\langle 0 | [\mathbf{H}, \hat{\phi}]\hat{\phi} | 0 \rangle = \left(\langle 0 | \mathbf{H}\hat{\phi} - \langle 0 | \hat{\phi}\mathbf{H} \right) \hat{\phi} | 0 \rangle = \langle 0 | \hat{\phi}(E_0 - \mathbf{H})\hat{\phi} | 0 \rangle.$$

Exchanging \hat{k} and \hat{k}' in the second expression ($W^{(2)}$ is symmetric) and taking the half difference, one concludes

$$\langle 0 | \hat{\phi}(\hat{k})(\mathbf{H} - E_0)\hat{\phi}(\hat{k}') | 0 \rangle = \frac{1}{2}[\hat{\phi}(\hat{k}), [\mathbf{H}, \hat{\phi}(\hat{k}')]].$$

Thus,

$$\delta^{d-1}(\hat{k} + \hat{k}') \left. \frac{\partial}{\partial t} W^{(2)}(\hat{k}, t) \right|_{t \rightarrow 0_+} = -\frac{1}{2}(2\pi)^{d-1} \langle 0 | [\hat{\phi}(\hat{k}), [\mathbf{H}, \hat{\phi}(\hat{k}')]] | 0 \rangle.$$

If the Hamiltonian density has the form (5.25), classical fields being replaced by quantum operators,

$$\mathbf{H}(\hat{\pi}, \hat{\phi}) = \frac{1}{2} \hat{\pi}^2(x) + \frac{1}{2} \left(\nabla \hat{\phi}(x) \right)^2 + V(\hat{\phi}(x)),$$

the commutator is proportional to the conjugated momentum:

$$[\mathbf{H}, \hat{\phi}(\hat{k})] = \int \frac{d^{d-1}x}{(2\pi)^{d-1}} e^{-i\hat{k}x} [\mathbf{H}, \hat{\phi}(x)] = -i \int \frac{d^{d-1}x}{(2\pi)^{d-1}} e^{-i\hat{k}x} \hat{\pi}(x).$$

Then,

$$[\hat{\phi}(\hat{k}), [\mathbf{H}, \hat{\phi}(\hat{k}')]] = (2\pi)^{1-d} \delta^{d-1}(\hat{k} + \hat{k}').$$

It follows that

$$\left. \frac{\partial}{\partial t} W^{(2)}(t, \hat{k}) \right|_{t \rightarrow 0_+} = -\frac{1}{2}.$$

Comparing this result with equation (5.64), we infer

$$\int d\alpha \rho(\alpha) = 1.$$

Since by definition the physical mass m is the lowest energy eigenstate above the ground state, the support of ρ is $\alpha \geq m$. Moreover, at $\hat{k} = 0$ the state is isolated. Therefore, the measure has an isolated δ -function and then a continuous part starting at the threshold for scattering states ($M = 3m$ in the simple ϕ^4 scalar field theory).

$$\rho(\alpha) = Z\delta(\alpha - m) + \rho'(\alpha), \quad \rho'(\alpha) = 0 \text{ for } m < \alpha < M. \quad (5.66)$$

We conclude that, except in a free field theory, the residue Z of the pole at $p^2 = -m^2$, is strictly smaller than 1:

$$0 < Z < 1.$$

5.11.3 Implications

This result has several implications, one being related to the S -matrix. Let us evaluate $W^{(2)}(t, \hat{k})$ for t large. The state of lowest energy, with momentum \hat{k} , gives the leading contribution. From the KL representation (5.63) and the decomposition (5.66), we then learn that

$$W^{(2)}(t, \hat{k}) \underset{t \rightarrow \infty}{\sim} \frac{Z}{2\sqrt{\hat{k}^2 + m^2}} e^{-|t|\sqrt{\hat{k}^2 + m^2}}.$$

If we compare this result with the contribution of a normalized one-particle eigenstate of the Hamiltonian \mathbf{H}_0 (see equation (5.43)),

$$(2\pi)^{d-1} \langle 1, \hat{k} | e^{-|t|(\mathbf{H} - E_0)} | 1, \hat{k}' \rangle = \delta^{d-1}(\hat{k} + \hat{k}') \frac{1}{2\sqrt{\hat{k}^2 + m^2}} e^{-|t|\sqrt{\hat{k}^2 + m^2}},$$

we observe that the field ϕ has only a component \sqrt{Z} on the one-particle states.

Another way to formulate the same result is to verify that in real time the Heisenberg field has a free field large time behaviour with an amplitude \sqrt{Z} on normalized creation or annihilation operators. After continuation to real time, one finds the two-point function

$$\begin{aligned} \langle 0 | \mathbf{T}[\hat{\phi}(t, \hat{k}) \hat{\phi}(0, \hat{k}')] | 0 \rangle &= \langle 0 | \hat{\phi}(\hat{k}) e^{-i(\mathbf{H}-E_0)|t|} \hat{\phi}(\hat{k}') | 0 \rangle \\ &= (2\pi)^{1-d} \delta^{d-1}(\hat{k} + \hat{k}') \int d\mu \frac{\rho(\mu)}{2\sqrt{\hat{k}^2 + \mu^2}} e^{-i|t|\sqrt{\hat{k}^2 + \mu^2}}. \end{aligned}$$

It can be verified that its large time behaviour is related to the leading singularity of the measure ρ . Since $\rho(\mu)$ is the sum of a δ -function and a continuous function (for $d \geq 2$), one obtains

$$\langle 0 | \hat{\phi}(\hat{k}) e^{-i(\mathbf{H}-E_0)|t|} \hat{\phi}(\hat{k}') | 0 \rangle \underset{|t| \rightarrow \infty}{=} (2\pi)^{1-d} \delta^{d-1}(\hat{k} + \hat{k}') \frac{Z e^{-i\omega(\hat{k})|t|}}{2\omega(\hat{k})} + O(1/t).$$

Introducing $\varphi, \bar{\varphi}$, the properly normalized creation and annihilation operators of the one-particle states, we conclude that for large time the field $\hat{\phi}(t, \hat{k})$ tends in a weak sense (not in an operator sense, but in all expectation values) towards

$$\hat{\phi}(t, \hat{k}) \underset{|t| \rightarrow \infty}{\sim} \sqrt{Z} \frac{1}{2\omega(\hat{k})} \left[\varphi(-\hat{k}) + \bar{\varphi}(\hat{k}) \right].$$

The constant \sqrt{Z} is the **field renormalization constant**.

Normalized S-matrix elements. To calculate properly normalized S -matrix elements we can calculate with the action $\mathcal{A}(\phi\sqrt{Z})$. Alternatively, if we keep the initial field we have to renormalize the matrix elements.

5.12 The non-relativistic limit

Since a general discussion of the non-relativistic limit of quantum field theory would be somewhat involved, we consider here only one example that illustrates the main point. We show that the low-energy limit of relativistic quantum field theory for massive particles is **many-body** quantum mechanics, and leads to a formalism naturally adapted to the **statistical physics of non-relativistic quantum particles**.

The ϕ^4 interaction. We consider a massive scalar field theory with a ϕ^4 type interaction. To discuss the non-relativistic limit, it is convenient to employ the real time formalism. The real-time evolution operator is given by a functional integral of the form

$$U = \int [d\phi] \exp i\mathcal{A}(\phi),$$
$$\mathcal{A}(\phi) = \int dt dx \left[\frac{1}{2} (\dot{\phi}(t, x))^2 - \frac{1}{2} (\nabla_x \phi(t, x))^2 - \frac{1}{2} m^2 \phi^2(t, x) - \frac{1}{4!} g \phi^4(t, x) \right].$$

At least for a coupling weak enough, the integral is dominated by fields satisfying the free field equation

$$(\partial_t^2 - \nabla_x^2 + m^2) \phi(t, x) = 0.$$

In the non-relativistic limit the space variation is small compared to the time variation. If space variations are completely neglected, the solutions to the field equation reduce simply to $\phi(t, x) \propto e^{\pm imt}$. It is thus natural to introduce the holomorphic representation of fields, taking as the unperturbed harmonic oscillator $\mathcal{A}_0(\phi)$:

$$\mathcal{A}_0(\phi) = \int dt dx \left[\frac{1}{2} (\dot{\phi}(t, x))^2 - \frac{1}{2} m^2 \phi^2(t, x) \right].$$

Denoting by $\varphi(t, x), \bar{\varphi}(t, x)$ the complex fields, in terms of which the field $\phi(t, x)$ reads

$$\phi(t, x) = (2m)^{-1/2} (\varphi(t, x) + \bar{\varphi}(t, x)),$$

one finds the action

$$\begin{aligned} \mathcal{A}(\varphi, \bar{\varphi}) &= \int dt dx \left[-i\bar{\varphi}\dot{\varphi} - m\varphi\bar{\varphi} - \frac{1}{4m} (\nabla_x (\varphi + \bar{\varphi}))^2 - \frac{g}{96m^2} (\varphi + \bar{\varphi})^4 \right]. \end{aligned}$$

To separate the fast time frequencies, one then takes new field variables

$$\varphi(t, x) \mapsto e^{imt} \varphi(t, x), \quad \bar{\varphi}(t, x) \mapsto e^{-imt} \bar{\varphi}(t, x),$$

where the new fields $\bar{\varphi}, \varphi$ have slow time variation compared to the factors e^{imt} .

After this transformation, the monomials of the form $\bar{\varphi}^r \varphi^s$ are multiplied by a factor $e^{im(s-r)t}$. For $r \neq s$ the corresponding time integrals give small contributions due to the rapid time oscillations. Hence, at leading order, the only surviving terms are those that have an equal number of $\bar{\varphi}$ and φ factors. The action, at leading order in the non-relativistic limit, reduces to

$$\mathcal{A}(\bar{\varphi}, \varphi) = \int dt dx \left(-i\varphi\dot{\bar{\varphi}} - \frac{1}{2m} \nabla_x \varphi \nabla_x \bar{\varphi} - \frac{g}{16m^2} \varphi\varphi\bar{\varphi}\bar{\varphi} \right).$$

We recognize a real-time action written in terms of complex fields of the form (5.22). Therefore, the Hamiltonian in the non-relativistic limit commutes with the particle number. This property, in general, is shared in relativistic quantum field theory only by free Hamiltonians. By contrast, in the non-relativistic limit of a massive theory all momenta are small compared to masses and, therefore, the number of particles is necessarily conserved.

Up to an infinite energy shift (the vacuum energy), the n -particle Hamiltonian H_n has the form

$$H_n = -\frac{1}{2m} \sum_{i=1}^n \nabla_{x_i}^2 + \frac{g}{8m^2} \sum_{i < j \leq n} \delta(x_i - x_j).$$

This is an n -particle Hamiltonian with two-body δ -function repulsive forces.

Finally, note that if we had expanded the fields with respect to the true physical mass, which is equal to m only for $g = 0$, we would have generated an additional chemical potential.

This analysis shows that the low-energy, non-relativistic limit of relativistic quantum field theory is many-body quantum mechanics in the second quantization formulation.