Advanced Quantum Field Theory (2024/2025)
TP 1 - Partition function of a real massless scalar field

In this session we review the canonical quantization procedure, introduced in the first course on Quantum Field Theory, using the example of a real massless scalar field. We will first study the system in finite volume, compute its free energy, and subsequently study its properties in the large volume approximation.

Exercise 1

Consider a real massless scalar field in $d+1$ dimensions, whose action is (using the mostly plus convention for the Minkowski metric)

$$S = \int dt\, d^d x \mathcal{L} = -\int dt\, d^d x \frac{1}{2}(\partial_\mu \phi)(\partial^\mu \phi). \tag{1}$$

We will quantize the system in a d-dimensional box with length $2L_i$ in i-th spatial direction ($i = 1, \ldots, d$), imposing periodic boundary conditions.

1. In order to perform the canonical quantization we will first construct the Hamiltonian for the action (1). Determine the momentum $\pi(x)$ of the scalar field and perform a Legendre transformation on the Lagrangian to find for the Hamiltonian

$$H = \int d^3 x \left(\frac{1}{2}\pi^2 + \frac{1}{2}(\partial_i \phi)(\partial^i \phi) \right). \tag{2}$$

In canonical quantization the Poisson brackets between field ϕ and momentum π of the classical theory become the fundamental equal-time commutation relations for the corresponding quantum operators

$$[\hat{\phi}(t,\vec{x}), \hat{\pi}(t,\vec{y})] = i\delta(\vec{x}-\vec{y}), \qquad [\hat{\phi}(t,\vec{x}), \phi(t,\vec{y})] = [\hat{\pi}(t,\vec{x}), \pi(t,\vec{y})] = 0, \tag{3}$$

Working on an initial time surface $t = 0$, we can expand ϕ in Fourier modes

$$\phi(t=0, x^i) = \sum_{\{k_1\}} \cdots \sum_{\{k_d\}} \phi(k_1, \ldots, k_d) e^{ik_i x^i} \equiv \sum_{\{k_i\}} \phi_{\{k_i\}} e^{ik_i x^i}, \tag{4}$$

where the sums range over all allowed values of the momenta.

2. Why do the momenta take on discrete values so that we have a sum (in contrast to an integral) over the allowed momenta? What is the range of allowed momenta over which the sums are to be performed?

3. What constraint on the coefficients $\phi_{\{k_i\}}$ is imposed by the reality condition on ϕ?

4. Invert the relationship (4) to obtain the modes in terms of the field ϕ.

5. Show that

$$\int d^d x f(x) g(x) = V \sum_{\{n_i\}} f_{\{k_i\}} g^*_{\{k_i\}}, \tag{5}$$

where f and g are two real functions admitting the expansion (4) and V is the volume of the box, and use this result to proved that the Hamiltonian (2) takes the form

$$H = \frac{V}{2} \sum_{\{n_i\}} \left(\pi_{k_i} \pi^*_{k_i} + \omega^2 \phi_{k_i} \phi^*_{k_i} \right) , \tag{6}$$

where π_{k_i} are the expansion coefficients of $\phi(x)$ and $\omega^2 = k^i k_i$.

6. We are now in the position to quantize the theory. Both position and momentum are promoted to operators that obey the commutation relations (3). Similarly, their Fourier coefficients $\hat{\phi}_{k_i}, \hat{\pi}_{k_i}$ are also promoted to operators. Use the commutation relations to show that

$$[\hat{\phi}_{k_i}, \hat{\pi}^*_{k'_i}] = \frac{i}{V} \delta_{k_i,k'_i} \qquad [\hat{\pi}_{k_i}, \hat{\pi}^*_{k'_i}] = [\hat{\phi}_{k_i}, \hat{\phi}^*_{k'_i}] = 0. \tag{7}$$

From now on we will ignore the zero mode corresponding to $k_i = 0, \forall i$ in the Fourier expansion. The contribution of this mode has to be treated separately and will be subleading in the large volume approximation. We will use $\sum'$ to indicate the sum without the inclusion of the zero mode.

7. Introduce the raising and lowering operators $a^\dagger_{k_i}$ and a_{k_i} by

$$a_{k_i} \equiv \sqrt{\frac{\omega_k V}{2}} \left(\phi_{k_i} + \frac{i}{\omega_{k_i}} \pi_{k_i} \right) \tag{8}$$

$$a^\dagger_{k_i} \equiv \sqrt{\frac{\omega_k V}{2}} \left(\phi^*_{k_i} - \frac{i}{\omega_{k_i}} \pi^*_{k_i} \right) , \tag{9}$$

where for brevity we dropped the hats from ϕ_{k_i} and π_{k_i}. Prove that these operators obey

$$[a_{k_i}, a^\dagger_{k'_i}] = \delta_{k_i,k'_i} \qquad [a_{k_i}, a_{k'_i}] = [a^\dagger_{k_i}, a^\dagger_{k'_i}] = 0 \,. \tag{10}$$

8. Invert the relations (8) to express ϕ_{k_i} and π_{k_i} in terms of creation and annihilation operator. Use this result in (6) to write the Hamiltonian as a collection of independent harmonic oscillators. After normal ordering the result, you should find

$$H = {\sum_{\{n_i\}}}' \omega_{k_i} a^\dagger_{k_i} a_{k_i} \,. \tag{11}$$

9. Choosing a convenient basis, compute the partition function of the theory at finite temperature $1/\beta$, defined as

$$Z(\beta) = \mathrm{Tr} e^{-\beta H} \,. \tag{12}$$

After taking the logarithm, you should find

$$\log Z(\beta) = - {\sum_{\{n_i\}}}' \log(1 - e^{-\beta \omega_{k_i}}) \,. \tag{13}$$

10. In the large volume limit, show that we can replace the sums in (13) by $\sum_{\{n_i\}} \to V/(2\pi)^d \int d^d k$. Perform the resulting integral. You should find

$$\log Z(\beta) = \frac{V}{(2\pi)^d} \frac{2\pi^{d/2}}{\Gamma(d/2)} \beta^{-d} \frac{1}{d} \Gamma(d+1) \zeta(d+1) \,. \tag{14}$$

Here, $\Gamma(s)$ denotes the Gamma function with the properties

$$\Gamma(s+1) = s\Gamma(s), \qquad \Gamma(n+1) = n! \qquad \forall n \in \mathbb{N} \qquad \Gamma(1/2) = \sqrt{\pi} \tag{15}$$

and $\zeta(s)$ is the Riemann zeta function defined as

$$\zeta(s) \equiv \sum_{n=1}^{\infty} \frac{1}{n^s} = \frac{1}{\Gamma(s)} \int_0^{\infty} dz \frac{z^{s-1}}{e^z - 1} \,. \tag{16}$$

You might also need the area of an $(n-1)$-sphere, which is given by

$$\Omega_{n-1} = \frac{2\pi^{n/2}}{\Gamma(n/2)} \,. \tag{17}$$

11. Evaluate the partition function (14) for the specific cases of $d = 1, 2, 3$. The corresponding values for the zeta function are $\zeta(2) = \frac{\pi^2}{6}, \zeta(4) = \frac{\pi^4}{90}$. For $\zeta(3)$ we have $\zeta(3) \approx 1.20$.

12. Having derived the partition function we can use it to determine macroscopic thermodynamic quantities. From $F(\beta) = -\beta^{-1} \log Z(\beta)$ we find

$$p = \beta^{-1} \frac{\partial \log Z(\beta)}{\partial V} \qquad \epsilon = -V^{-1} \frac{\partial \log Z(\beta)}{\partial \beta} \tag{18}$$

for pressure p and energy density ϵ. Show that the equation of state $\epsilon = 3p$ for a relativistic gas in $d = 3$ holds.

13. The energy density of black body radiation (three-dimensional gas of massless photons) is given by the Stefan–Boltzmann law

$$\epsilon_{BB} = 4\sigma_{SB}\beta^{-4} = \frac{\pi^2}{15}\beta^{-4} \,. \tag{19}$$

Compare this result with the one you found in 12. How and why do these results differ?

Exercise 2

In this exercise we are going to mirror the computation of the previous exercise, but now for a scalar field obeying different boundary conditions. For simplicity, we will restrict ourselves to a $1+1$-dimensional system.

Consider a real massless scalar field in $1+1$ dimensions on an interval of length L with boundary conditions

$$\phi(0) = \phi(L) = 0 \,. \tag{20}$$

1. Write down a convenient Fourier expansion of the fields. What constraint on the Fourier coefficients is imposed by the reality condition? Which values does the momentum k take?

2. We will from now on use the expansion

$$\phi(x) = \sqrt{2} \sum_{n>0}^{\infty} \phi_k \sin(kx) \,, \tag{21}$$

where the factor of $\sqrt{2}$ was introduced for later convenience. Invert the relation (21) to obtain ϕ_k in terms of ϕ. You may find useful the following integral

$$\int_0^{\pi} \sin(mz)\sin(nz) = \frac{\pi}{2}\delta_{m,n} \qquad m, n \in \mathbb{Z} \,. \tag{22}$$

3. Show that

$$\int_0^L dx f(x) g(x) = L \sum_{n>0} f_k g_k, \tag{23}$$

where f and g are two real function admitting the expansion (21).

4. Use this result to write the Hamiltonian (2) in terms of the modes ϕ_k, π_k. You should find

$$H = \frac{L}{2} \sum_{n>0} (\pi_k^2 + \omega_k^2 \phi_k^2) \qquad \omega_k^2 = k^2 \,. \tag{24}$$

5. Using the canonical commutation relations (3), prove that

$$[\hat{\phi}_{k_i}, \hat{\pi}^*_{k'_i}] = \frac{i}{L} \delta_{k_i, k'_i} \qquad [\hat{\pi}_{k_i}, \hat{\pi}^*_{k'_i}] = [\hat{\phi}_{k_i}, \hat{\phi}^*_{k'_i}] = 0. \tag{25}$$

6. Define the raising and lowering operators

$$a_{k_i} \equiv \sqrt{\frac{\omega_k V}{2}} \left(\phi_{k_i} + \frac{i}{\omega_{k_i}} \pi_{k_i} \right) \tag{26}$$

$$a^\dagger_{k_i} \equiv \sqrt{\frac{\omega_k V}{2}} \left(\phi_{k_i} - \frac{i}{\omega_{k_i}} \pi_{k_i} \right) , \tag{27}$$

and prove that

$$[a_k, a^\dagger_{k'}] = \delta_{k,k'} \qquad [a^\dagger_k, a^\dagger_{k'}] = [a_k, a_{k'}] = 0 \,. \tag{28}$$

7. Invert the relations (26) to express the Hamiltonian as a collection of independent harmonic oscillators. After normal ordering you should find

$$H = \sum_{n>0} \omega_k a^\dagger_k a_k \,. \tag{29}$$

8. Choosing a convenient basis, compute the partition function of the theory at finite temperature β^{-1}, defined as

$$Z(\beta) = \mathrm{Tr} e^{-\beta H} \,. \tag{30}$$

After taking the logarithm, you should find

$$\log Z(\beta) = - \sum_{n>0} \log(1 - e^{-\beta \omega_k}) \qquad \omega_k = \frac{n\pi}{L} \,. \tag{31}$$

9. Take the limit of large volume to approximate the sum in (31) as a continuous integral. Use integration by parts to get the final result

$$\log Z(\beta) = \frac{V\pi}{6} \beta^{-1} \qquad V = L \,. \tag{32}$$

Compare this with the one you found in the first exercise. You will conclude that the bulk partition function computed in the large volume approximation does not depend on the boundary conditions.