Classical and quantum scalar field

Our introduction to statistical quantum field theory will mostly deal with scalar real fields. So, let's start with a reminder of the classical free scalar field and its canonical quantization.

Classical description of a scalar field

- The fundamental quantity of classical and quantum field theory is the action S defined through the Lagrangian density $\mathcal{L}(x)$ as

$$S \equiv \int d^4x \, \mathcal{L}. \tag{1}$$

- The Lagrangian density of noninteracting scalar field $\phi(x)$ is

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

  where m is the mass parameter. The field is assumed to be real.

- Since the action S is dimensionless, $\mathcal{L}$ is of the dimension m^4 and consequently the field ϕ is of the dimension m.

- The principle of the minimal action leads to the Eulera-Lagrange equation

$$\partial^\mu \frac{\partial \mathcal{L}}{\partial(\partial^\mu \phi)} - \frac{\partial \mathcal{L}}{\partial \phi} = 0, \tag{3}$$

  which gives the Klein-Gordon equation

$$\left[\partial_\mu \partial^\mu + m^2\right] \phi(x) = 0 \tag{4}$$

  for the Lagrangian density (2).

- There is no conserved charge carried by the real field.

- One asks how $\phi(x)$ transforms under the Lorentz transformation?

- To answer this question one postulates that the field $\phi(x)$ satisfies the Klein-Gordon equation in any reference frame.

- If $\phi(x) \to \phi'(x')$, then

$$\left[\partial'_\mu \partial'^\mu + m^2\right] \phi'(x') = 0, \tag{5}$$

  where m is assumed to be Lorentz invariant.

- Since $\partial'_\mu \partial'^\mu = \partial_\mu \partial^\mu$, we find

$$\phi(x) \to \phi'(x') = \phi(\Lambda^{-1} x'), \tag{6}$$

  where Λ is the transformation matrix of four-vectors that is $x'^\mu = \Lambda^\mu{}_\nu x^\nu$.

- The field which transforms according to the rule (6) is called scalar.

- One arrives to the same transformation rule (6) postulating that the Lagrangian density (2) is a Lorentz invariant or Lorentz scalar.

- To perform the canonical quantization we need to formulate the Hamiltonian or canonical formalism. For this reason we define the canonical momentum $\pi(x)$ conjugate to $\phi(x)$ as

$$\pi(x) \equiv \frac{\partial \mathcal{L}(x)}{\partial \dot{\phi}(x)} = \dot{\phi}(x), \tag{7}$$

where the dot denotes the time derivative.

- The equal-time Poisson bracket of quantities $A(x)$ and $B(x)$ is

$$\{A(t,\mathbf{x}), B(t,\mathbf{x}')\}_{\rm PB} \equiv \int d^3x'' \bigg(\frac{\delta A(t,\mathbf{x})}{\delta \phi(t,\mathbf{x}'')}\frac{\delta B(t,\mathbf{x}')}{\delta \pi(t,\mathbf{x}'')} - \frac{\delta A(t,\mathbf{x})}{\delta \pi(t,\mathbf{x}'')}\frac{\delta B(t,\mathbf{x}')}{\delta \phi(t,\mathbf{x}'')}\bigg), \tag{8}$$

where the functional differentiation is done according to standard rules of differentiation supplemented by the rule

$$\frac{\delta f(t,\mathbf{x})}{\delta f(t,\mathbf{x}')} = \delta^{(3)}(\mathbf{x}-\mathbf{x}'). \tag{9}$$

The time t is not treated as a variable of differentiated function but as a parameter.

- One easily checks that the Poisson bracket of the pair of canonical variables $\phi(x)$ and $\pi(x)$ is

$$\{\phi(t,\mathbf{x}), \pi(t,\mathbf{x}')\}_{\rm PB} = \delta^{(3)}(\mathbf{x}-\mathbf{x}'), \tag{10}$$

and

$$\{\phi(t,\mathbf{x}), \phi(t,\mathbf{x}')\}_{\rm PB} = \{\pi(t,\mathbf{x}), \pi(t,\mathbf{x}')\}_{\rm PB} = 0. \tag{11}$$

- The Hamiltonian density $\mathcal{H}$ is defined by means of the Legendre transformation

$$\mathcal{H}(x) \equiv \pi(x)\,\dot{\phi}(x) - \mathcal{L}(x) \tag{12}$$

and the Hamiltonian equals

$$H = \int d^3x\,\mathcal{H}(x). \tag{13}$$

- Using the Lagrangian density (2), one finds

$$\mathcal{H}(x) = \frac{1}{2}\pi^2(x) + \frac{1}{2}(\nabla\phi(x))^2 + \frac{1}{2}m^2\phi^2(x). \tag{14}$$

- The canonical equations of motion are

$$\dot{\phi}(x) = \frac{\delta H}{\delta \pi(x)} = \pi(x), \tag{15}$$

$$\dot{\pi}(x) = -\frac{\delta H}{\delta \phi(x)} = \left(\nabla^2 - m^2\right)\phi(t,\mathbf{x}). \tag{16}$$

The first equation determines the relation between the canonical momentum $\pi(x)$ and the position $\phi(x)$ while the first one combined with the second one gives the Klein-Gordon equation (4).

- The canonical equations of motion can be written by means of the Poisson brackets as

$$\dot{\phi}(t,\mathbf{x}) = \{\phi(t,\mathbf{x}), H\}_{\rm PB} = \pi(t,\mathbf{x}), \tag{17}$$

$$\dot{\pi}(t,\mathbf{x}) = \{\pi(t,\mathbf{x}), H\}_{\rm PB} = \left(\nabla^2 - m^2\right)\phi(t,\mathbf{x}). \tag{18}$$

- The plane-wave solution of the Klein-Gordon equation is written as

$$\phi(x) = \int \frac{d^3k}{(2\pi)^3\sqrt{2\omega_{\mathbf{k}}}} \Big[e^{-ikx}a(\mathbf{k}) + e^{ikx}a^*(\mathbf{k})\Big], \tag{19}$$

  where $k^\mu = (\omega_{\mathbf{k}}, \mathbf{k})$ with $\omega_{\mathbf{k}} \equiv \sqrt{m^2 + \mathbf{k}^2}$, and $a(\mathbf{k})$ is unknown complex valued function of the dimension $m^{-3/2}$.

- One checks that the field (19) is real that is $\phi^*(x) = \phi(x)$.

- The solution (19) has been written in the form which guarantees that the Hamiltonian (13) obtained from the Hamiltonian density (14) is

$$H = \int \frac{d^3k}{(2\pi)^3}\, \omega_{\mathbf{k}}\, a(\mathbf{k})\, a^*(\mathbf{k}). \tag{20}$$

- The Hamiltonian (20) is obviously nonnegative. Consequently, the total system's energy is nonnegative even so there seem to be the negative energy components in the solution (19).

Exercise: Derive the formula (20).

Quantization of scalar field

- The classical field $\phi(x)$ and its conjugate momentum $\pi(x)$ are replaced by the operators $\hat\phi(x)$ and $\hat\pi(x)$ that is

$$\begin{aligned} \phi(x) &\longrightarrow \hat\phi(x), \\ \pi(x) &\longrightarrow \hat\pi(x). \end{aligned}$$

  The operators act in the space of states also called the Fock space.

- We postulate the equal-time commutation relations

$$[\hat\phi(t,\mathbf{x}), \hat\pi(t,\mathbf{x}')] = i\hbar\delta^{(3)}(\mathbf{x}-\mathbf{x}'), \tag{21}$$

$$[\hat\phi(t,\mathbf{x}), \hat\phi(t,\mathbf{x}')] = 0, \tag{22}$$

$$[\hat\pi(t,\mathbf{x}), \hat\pi(t,\mathbf{x}')] = 0, \tag{23}$$

  which are obtained by replacing the Poisson brackets (10, 11) by the commutators multiplied by $-\frac{i}{\hbar}$ that is

$$\{\dots,\dots\}_{\rm PB} \longrightarrow -\frac{i}{\hbar}[\dots,\dots].$$

- Further on we use the natural units where $\hbar = 1$.

- The field operator $\hat\phi(x)$, which obeys the Klein-Gordon equation

$$[\partial_\mu\partial^\mu + m^2]\,\hat\phi(x) = 0, \tag{24}$$

  is written analogously to its classical counterpart (19) as

$$\hat\phi(x) = \int \frac{d^3k}{(2\pi)^3\sqrt{2\omega_{\mathbf{k}}}} \Big[e^{-ikx}\hat a(\mathbf{k}) + e^{ikx}\hat a^\dagger(\mathbf{k})\Big], \tag{25}$$

  where $\hat a(\mathbf{k})$ and $\hat a^\dagger(\mathbf{k})$ are the annihilation and creation operators and $\dagger$ denotes the Hermitian conjugation.

- The commutation relations (21, 22, 23) lead to the commutation relations of $\hat{a}(\mathbf{k})$ and $\hat{a}^\dagger(\mathbf{k})$

$$\begin{aligned}[\hat{a}(\mathbf{k}), \hat{a}^\dagger(\mathbf{k}')] &= (2\pi)^3 \delta^{(3)}(\mathbf{k} - \mathbf{k}'), &(26)\\ [\hat{a}(\mathbf{k}), \hat{a}(\mathbf{k}')] &= 0, &(27)\\ [\hat{a}^\dagger(\mathbf{k}), \hat{a}^\dagger(\mathbf{k}')] &= 0. &(28)\end{aligned}$$

- Eqs. (21, 22, 23) almost immediately follow from Eqs. (26, 27, 28). The proof of the inverse theorem is more difficult.

Exercise: Derive Eqs. (21, 22, 23) from Eqs. (26, 27, 28).

Exercise: Derive Eqs. (26, 27, 28) from Eqs. (21, 22, 23).

- Since the operators $\hat{a}(\mathbf{k})$ and $\hat{a}^\dagger(\mathbf{k})$ do not commute with each other, the quantum analogue of the classical Hamiltonian (20) is

$$\hat{H} = \int \frac{d^3k}{(2\pi)^3} \frac{\omega_{\mathbf{k}}}{2} \Big(\hat{a}(\mathbf{k})\, \hat{a}^\dagger(\mathbf{k}) + \hat{a}^\dagger(\mathbf{k})\, \hat{a}(\mathbf{k})\Big). \tag{29}$$

- The construction of a space of states, which is discussed later on, is much simplified if the continuous momentum $\mathbf{k}$ is replaced by a set of discrete values $\{\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3, \dots\}$. So, we assume that the field is periodic with the period L in every direction that is

$$\hat{\phi}(t, \mathbf{x}) = \hat{\phi}(t, \mathbf{x} + \mathbf{e}_k L), \qquad k = 1,\, 2,\, 3, \tag{30}$$

  where $\mathbf{e}_1 = (1, 0, 0)$, $\mathbf{e}_2 = (0, 1, 0)$, $\mathbf{e}_3 = (0, 0, 1)$.

- The field (25) satisfies the condition (30) if $e^{\pm i\mathbf{k}\cdot\mathbf{e}_k L} = 1$. Consequently, $\mathbf{k}$ takes the discrete values

$$\mathbf{k}_{n_1,n_2,n_3} = \frac{2\pi}{L}(n_1, n_2, n_3), \qquad n_k = 0,\, \pm 1,\, \pm 2,\, \dots \tag{31}$$

- When the discrete values of $\mathbf{k}$ are used, the integrals over $\mathbf{k}$ are changed into the sums and the Dirac deltas into the Kronecker deltas

$$\int \frac{d^3k}{(2\pi)^3} \cdots \to \frac{1}{L^3} \sum_i \cdots, \qquad (2\pi)^3 \delta^{(3)}(\mathbf{k} - \mathbf{k}') \to L^3 \delta^{ij}, \tag{32}$$

  where the triple index (n_1, n_2, n_3) is replaced by the index i.

- We introduce the dimensionless creation and annihilation operators as

$$\hat{a}_i \equiv \frac{1}{\sqrt{L^3}}\, \hat{a}(\mathbf{k}_i), \qquad \hat{a}_i^\dagger \equiv \frac{1}{\sqrt{L^3}}\, \hat{a}^\dagger(\mathbf{k}_i), \tag{33}$$

  which obey the relations

$$\begin{aligned}[\hat{a}_i, \hat{a}_j^\dagger] &= \delta^{ij}, &(34)\\ [\hat{a}_i, \hat{a}_j] &= 0, &(35)\\ [\hat{a}_i^\dagger, \hat{a}_j^\dagger] &= 0, &(36)\end{aligned}$$

  obtained from Eqs. (26, 27, 28).

- The Hamiltonian (29) becomes

$$\hat{H} = \sum_i \frac{\omega_i}{2}\left(\hat{a}_i\,\hat{a}_i^\dagger + \hat{a}_i^\dagger\,\hat{a}_i\right) = \sum_i \omega_i\Big(\hat{a}_i^\dagger\,\hat{a}_i + \frac{1}{2}\Big), \tag{37}$$

where $\omega_i \equiv \sqrt{\mathbf{k}_i^2 + m^2}$.

- The formula (37) shows that the system's energy is a sum of energies of independent harmonic oscillators.

Construction of space of states

- We postulate an existence of an energy state $|E\rangle$ and using the annihilation operators we produce states of lower energies.
- Since the Hamiltonian (37) is positive definite there exists a state of the lowest energy $|0\rangle$ – the ground state which is called the vacuum state in the quantum field theory.
- An operator $\hat{A}$ is positive definite if

$$\langle\alpha|\hat{A}|\alpha\rangle \geqslant 0 \tag{38}$$

for any $|\alpha\rangle$.

- Since there is no state of the energy lower than that of $|0\rangle$, any annihilation operator $\hat{a}_i$ annihilates the state that is

$$\hat{a}_i|0\rangle = 0, \tag{39}$$

where the zero in the right-hand-side is the number zero.

- The Hermitian conjugate of Eq. (39) is

$$\langle 0|\hat{a}_i^\dagger = 0. \tag{40}$$

- The vacuum energy is

$$\langle 0|\hat{H}|0\rangle = \langle 0|\sum_i \omega_i\Big(\hat{a}_i^\dagger\,\hat{a}_i + \frac{1}{2}\Big)|0\rangle = \frac{1}{2}\sum_i \omega_i, \tag{41}$$

which, as the infinite sum of zero point energies $\omega_i/2$, is infinite.

- To eliminate the zero point infinite energy we introduce the normal ordering of operators which requires that annihilation operators are on the right hand side of creation operators.
- The normally ordered Hamiltonian (37) is

$$\hat{H} = \sum_i \omega_i \hat{a}_i^\dagger\,\hat{a}_i, \tag{42}$$

and $\langle 0|\hat{H}|0\rangle = 0$.

- The Fock space is spanned by the states of orthonormal basis $|n_1, n_2, n_3, \dots\rangle$ which are the energy and particle number eigenstates of the eigenvalues $\sum_i \omega_i n_i$ and $\sum_i n_i$, respectively. It means

$$\hat{H}|n_1, n_2, n_3, \dots\rangle = \Big(\sum_i \omega_i n_i\Big)|n_1, n_2, n_3, \dots\rangle, \tag{43}$$

$$\hat{N}|n_1, n_2, n_3, \dots\rangle = \Big(\sum_i n_i\Big)|n_1, n_2, n_3, \dots\rangle, \tag{44}$$

where $\hat{N} = \sum_i \hat{a}_i^\dagger \hat{a}_i$.

- The annihilation and creation operators act as

$$\hat{a}_i|n_1, n_2, \dots n_i, \dots\rangle = \sqrt{n_i}\,|n_1, n_2, \dots n_i - 1, \dots\rangle, \tag{45}$$

$$\hat{a}_i^\dagger|n_1, n_2, \dots n_i, \dots\rangle = \sqrt{n_i + 1}\,|n_1, n_2, \dots n_i + 1, \dots\rangle. \tag{46}$$

- The states $|n_1, n_2, n_3, \dots\rangle$ can be all obtained from the vacuum state as

$$|n_1, n_2, n_3, \dots\rangle = \frac{1}{\sqrt{n_1!\,n_2!\,n_3!}}(\hat{a}_1^\dagger)^{n_1}(\hat{a}_2^\dagger)^{n_2}(\hat{a}_3^\dagger)^{n_3}\dots|0\rangle. \tag{47}$$

- There can be an unlimited number of particles of a given momentum $\mathbf{k}_i$ in the state $|n_1, n_2, n_3, \dots\rangle$. Therefore, the real scalar field quantized by means of the commutation relations describes a system of <u>bosons</u> – particles which obey the Bose-Einstein statistics.