PH6418/ PH4618: Quantum Field Theory (Spring 2022)

Notes for Lecture 14-15: Quantization of the free scalar field*

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1 Recap of the classical theory

The theory of a classical relativistic scalar field is given by the action,

$$I\left[\varphi(x)\right] = \int d^4x\ \mathcal{L}(\varphi, \partial_\mu \varphi)$$

where the Lagrangian density $\mathcal{L}$ is a Lorentz scalar and a *local* function of the field, $\varphi(x)$ and its first order spacetime derivatives, $\partial_\mu \varphi(x)$. The physical reasons behind arriving at this type of action (lagrangian) has been outlined in the classical field theory course. This is a field theory, i.e. the generalized coordinates, $q_i(t)$ are labeled by a continuous label, namely the position/location of the coordinate, say $\varphi_{\boldsymbol{x}}(t)$ or better yet $\varphi(\boldsymbol{x}, t)$. The Euler-Lagrange equations of motion are given by,

$$\frac{\delta L}{\delta \varphi(\boldsymbol{x})} = \frac{d}{dt}\left(\frac{\delta L}{\delta \dot{\varphi}(\boldsymbol{x})}\right)$$

where $L = \int d^3\boldsymbol{x}\ \mathcal{L}$ is the Lagrangian. This equation is equivalent to the more familiar and relativistically covariant looking form,

$$\frac{\partial \mathcal{L}}{\partial \varphi} = \partial_\mu \left(\frac{\partial \mathcal{L}}{\partial\left(\partial_\mu \varphi\right)}\right). \tag{1}$$

The conjugate momentum field, say $\pi(\boldsymbol{x}, t)$

$$\pi(\boldsymbol{x}, t) = \frac{\delta L}{\delta \dot{\varphi}(\boldsymbol{x}, t)} = \frac{\partial \mathcal{L}}{\partial \dot{\varphi}(x)}.$$

The Hamiltonian for the theory can be derived from the Lagrangian via a Legendre transform,

$$H = \int d^3\boldsymbol{x}\, \pi(\boldsymbol{x}, t)\, \dot{\varphi}(\boldsymbol{x}, t) - L = \int d^3\boldsymbol{x}\ \mathcal{H}\left(\pi(x), \varphi(x)\right)$$

where $\mathcal{H}(x) = \pi(x)\dot{\varphi}(x) - \mathcal{L}(x)$ is the Hamiltonian density. Starting from the Hamiltonian one can also write down the Hamilton's equation of motion, namely,

$$\dot{\varphi}(\boldsymbol{x}, t) = \frac{\delta H}{\delta \pi(\boldsymbol{x}, t)}, \qquad \dot{\pi}(\boldsymbol{x}, t) = -\frac{\delta H}{\delta \varphi(\boldsymbol{x}, t)}.$$

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In general given a Hamiltonian for the scalar field, one can write down the evolution equation for a general field which is a function of both the scalar field, $\varphi(x)$ as well as its conjugate momentum field say $\mathcal{O}(\varphi(x), \pi(x))$ via the Poisson brackets equation,

$$\frac{d\mathcal{O}}{dt} = \{\mathcal{O}, H\}_{PB} \tag{2}$$

where the Poisson brackets are defined by the functional version for field theory,

$$\{A, B\}_{PB} = \int d^3\boldsymbol{x} \left(\frac{\delta A}{\delta\varphi(\boldsymbol{x}, t)} \frac{\delta B}{\delta\pi(\boldsymbol{x}, t)} - \frac{\delta B}{\delta\varphi(\boldsymbol{x}, t)} \frac{\delta A}{\delta\pi(\boldsymbol{x}, t)} \right). \tag{3}$$

In particular, the canonical Poisson brackets are,

$$\{\varphi(\boldsymbol{x}, t), \pi(\boldsymbol{y}, t)\}_{PB} = \delta^3(\boldsymbol{x} - \boldsymbol{y}), \tag{4}$$

$$\{\varphi(\boldsymbol{x}, t), \varphi(\boldsymbol{y}, t)\}_{PB} = \{\pi(\boldsymbol{x}, t), \pi(\boldsymbol{y}, t)\}_{PB} = 0. \tag{5}$$

The "free" theory is given by the particular Lagrangian density containing purely quadratic terms (Lorentz scalars)

$$\mathcal{L} = \frac{1}{2} (\partial_\mu\varphi) (\partial^\mu\varphi) - \frac{m^2}{2}\varphi^2.$$

The parameter m has the dimensions of mass, $[m] = 1$ and naturally called the mass parameter. However The equation of motion (1) is then linear in the field,

$$\left(\Box + m^2\right) \varphi(x) = 0, \tag{6}$$

where $\Box \equiv \partial^2 = \partial^\mu\partial_\mu$. The equation is called the Klein-Gordon equation, originally in the context of relativistic quantum mechanics with φ being a single particle (Schrödinger) wave-function, however here we are talking about a strictly classical field, $\varphi(x)$. Since for a linear equation of motion, for any two distinct solutions say $\varphi_1(x)$ and $\varphi_2(x)$ which satisfy the Klein-Gordon equation, any linear combination $\varphi(x) = c_1\varphi_1(x) + c_2\varphi_2(x)$, for arbitrary constants $c_{1,2}$ is also a solution (the superposition principle) i.e. the constituent fields, $\varphi_{1,2}$ do not mix with each other or scatter off each other, but evolve in time individually or separately. This lack of mixing of two solutions when superposed is why this theory is considered a noninteracting or free theory. The conjugate momentum is,

$$\pi(x) = \dot{\varphi}(x)$$

and the Hamiltonian is given by $H = \int d^3\boldsymbol{x}\, \mathcal{H}$,where the Hamiltonian density is,

$$\mathcal{H} = \frac{\dot{\varphi}^2}{2} + \frac{(\boldsymbol{\nabla}\varphi)^2}{2} + \frac{m^2\varphi^2}{2}.$$

From the expression of the Hamiltonian, we can write down the Hamilton's equations,

$$\dot{\varphi} = \pi, \qquad \dot{\pi} = -\boldsymbol{\nabla}^2\varphi + m^2\varphi,$$

combining which we again get the Klein-Gordon equation, $(\Box + m^2)\varphi(x) = 0$. The Klein-Gordon equation admits plane wave solutions, $\varphi(x) \sim e^{-ik.x}$ where $k = (\omega_{\boldsymbol{k}}, \boldsymbol{k})$ is the wave-vector and the dispersion relation,

$$\omega_{\boldsymbol{k}} = \sqrt{\boldsymbol{k}^2 + m^2}. \tag{7}$$

The general solution is given by the superposition of such (dispersive) plane waves,

$$\varphi(x) = \int \frac{d^3\boldsymbol{k}}{(2\pi)^2\, 2\omega_{\boldsymbol{k}}} \left(\varphi(\omega_{\boldsymbol{k}}, \boldsymbol{k})\, e^{-ik.x} + \text{c.c}\right), \tag{8}$$

where $\varphi(\omega_{\boldsymbol{k}}, \boldsymbol{k})$ is the amplitude for the component with wave-vector $k = (\omega_{\boldsymbol{k}}, \boldsymbol{k})$ and c.c. stands for "complex conjugate". Complex conjugation is necessary since the field is real.

1.1 Symmetries and conserved charges of the free theory

The free theory action is invariant under the the Poincaré symmetry,

$$x \to x' = \Lambda x + a$$

which is a group of continuous (i.e. the symmetry parameters are continuous variables taking values on $\mathbb{R}$or a subset of $\mathbb{R}$), global (since the symmetry parameters are same at all spacetime locations) symmetries. Then according to Noether's (first) theorem, there must exist a conserved Noether charge for each such continuous global symmetry parameter (c.f. Classical Field Theory notes for the Noether algorithm to extract charges from a continuous global symmetry of the action). For the translation symmetry, with symmetry parameters being components of the 4-vector, $a = (a^0, \boldsymbol{a})$, the conserved charges are the components of the momentum 4-vector, P^μ

$$P^0 = H = \int d^3\boldsymbol{x} \left(\frac{\dot{\varphi}^2}{2} + \frac{(\boldsymbol{\nabla}\varphi)^2}{2} + \frac{m^2\varphi^2}{2}\right), \tag{9}$$

$$\boldsymbol{P} = -\int d^3\boldsymbol{x}\, \pi\boldsymbol{\nabla}\varphi. \tag{10}$$

For the Lorentz symmetries (boosts and rotations) the conserved charges are the components of the rank 2 antisymmetric tensor $M^{\mu\nu}$,

$$M^{\mu\nu} = \int d^3\boldsymbol{x} \left(x^\mu T^{0\nu} - x^\nu T^{0\mu}\right)$$

where $T^{\mu\nu} = \partial^\mu\varphi \frac{\partial\mathcal{L}}{\partial(\partial_\nu\varphi)} - \eta^{\mu\nu}\varphi$ is the canonical stress-energy-momentum density tensor. (However these are only 3 charges, namely, the angular momentum charges, M^{ij}. The boost charges, $M^{0i} = x^0P^i - x_{CoM}P^0$, do not give rise to any new charges.)

There is also a discrete symmetry which is an internal symmetry, namely a global sign-flip in configuration space,

$$\varphi(x) \to -\varphi(x).$$

However since this is not a continuous symmetry there are no conserved Noether charges corresponding to this symmetry. However this discrete reflection symmetry will have a major consequence when we quantize the theory.

2 Quantizing the free (real) scalar theory: Canonical quantization

To quantize a field theory in general we will follow the *canonical quantization* procedure whereby we

1. Promote the coordinates and momenta to linear operators acting on a Hilbert space of states,

$$\varphi(x) \to \hat{\varphi}(x), \quad \pi(x) \to \hat{\pi}(x)$$

2. Promote the Poisson brackets of two classical functions (observables) to commutator of the respective operators

$$\{A, B\}_{PB} \to \frac{\left[\hat{A}, \hat{B}\right]}{i}.$$

In particular the canonical Poisson brackets (4-5) turn into the canonical commutation relations,

$$[\hat{\varphi}(\boldsymbol{x}, t), \hat{\pi}(\boldsymbol{y}, t)] = i\, \delta^3(\boldsymbol{x} - \boldsymbol{y}), \tag{11}$$

$$[\hat{\varphi}(\boldsymbol{x}, t), \hat{\varphi}(\boldsymbol{y}, t)] = [\hat{\pi}(\boldsymbol{x}, t), \hat{\pi}(\boldsymbol{y}, t)] = 0 \tag{12}$$

In terms of the 4-vectors, x, y

$$[\hat{\varphi}(x), \hat{\pi}(y)]_{x^0=y^0} = i\, \delta^3(\boldsymbol{x} - \boldsymbol{y}), \tag{13}$$

$$[\hat{\varphi}(x), \hat{\varphi}(y)]_{x^0=y^0} = [\hat{\pi}(x), \hat{\pi}(y)]_{x^0=y^0} = 0. \tag{14}$$

These are dubbed as the ***equal time canonical commutation relations*** **(ETCCR)**.

3. We work in the **Heisenberg picture** where the observables (operators) evolve in time but the state of the system does not evolve. To determine the quantum dynamics (evolution equation) of an observable, $\mathcal{O}$ we first promote it to an operator, $\hat{\mathcal{O}}$ (prescribed in step 1) and then by replace the Poisson brackets in the classical time evolution equation (2) by commutator brackets as prescribed in step 2:

$$\frac{d\hat{\mathcal{O}}}{dt} = \frac{\left[\hat{\mathcal{O}}, \hat{H}\right]}{i},$$

or,

$$\frac{d\hat{\mathcal{O}}}{dt} = i\left[\hat{H}, \hat{\mathcal{O}}\right] \tag{15}$$

This is the Heisenberg equation of motion.

****From here on since will be working with a quantum theory and every field or observable, say $\mathcal{O}$ appearing will be an operator, we will not bother to write the caret or hat, " ˆ ".****

Let's apply the procedure of canonical quantization to the free real scalar field theory introduced in the last section, $\varphi(x)$. The Hamiltonian is given by (9), and it is easy to check using the ETCCR's, that the evolution equation for the quantum field operators, $\varphi(x)$ and $\pi(x)$ are,

$$\begin{aligned}
\frac{\partial\varphi(\boldsymbol{x},t)}{\partial t} &= i\,[H,\varphi(\boldsymbol{x},t)] \\
&= i\,\left[\int d^3\boldsymbol{y}\;\mathcal{H}\left(\varphi(\boldsymbol{y},t),\pi(\boldsymbol{y},t)\right),\varphi(\boldsymbol{x},t)\right] \\
&= i\int d^3\boldsymbol{y}\,[\mathcal{H}\left(\varphi(\boldsymbol{y},t),\pi(\boldsymbol{y},t)\right),\;\varphi(\boldsymbol{x},t)] \\
&= \frac{i}{2}\int d^3\boldsymbol{y}\,\left[\pi^2(\boldsymbol{y},t),\;\varphi(\boldsymbol{x},t)\right] \\
&= i\int d^3\boldsymbol{y}\;\pi(\boldsymbol{y},t)\;\underbrace{[\pi(\boldsymbol{y},t),\;\varphi(\boldsymbol{x},t)]}_{=-\,i\,\delta^3(\boldsymbol{y}-\boldsymbol{x})} \\
\Rightarrow \pi(\boldsymbol{x},t) &= \frac{\partial\varphi(\boldsymbol{x},t)}{\partial t}, \qquad (16)
\end{aligned}$$

and,

$$\begin{aligned}
\frac{\partial\pi(\boldsymbol{x},t)}{\partial t} &= i\,[H,\pi(\boldsymbol{x},t)] \\
&= i\left[\int d^3\boldsymbol{y}\;\mathcal{H}\left(\varphi(\boldsymbol{y},t),\pi(\boldsymbol{y},t)\right),\;\pi(\boldsymbol{x},t)\right] \\
&= i\int d^3\boldsymbol{y}\,[\mathcal{H}\left(\varphi(\boldsymbol{y},t),\pi(\boldsymbol{y},t)\right),\;\pi(\boldsymbol{x},t)] \\
&= \frac{i}{2}\int d^3\boldsymbol{y}\,\left[\left(\boldsymbol{\nabla}_{\boldsymbol{y}}\varphi(\boldsymbol{y},t)\right)^2+m^2\,\varphi^2(\boldsymbol{y},t),\;\pi(\boldsymbol{x},t)\right] \\
&= i\int d^3\boldsymbol{y}\,\left(\boldsymbol{\nabla}_{\boldsymbol{y}}\varphi(\boldsymbol{y},t)\cdot\boldsymbol{\nabla}_y\left[\varphi(\boldsymbol{y},t),\;\pi(\boldsymbol{x},t)\right]+m^2\varphi(\boldsymbol{y},t)\;\left[\varphi(\boldsymbol{y},t),\;\pi(\boldsymbol{x},t)\right]\right) \\
\Rightarrow \frac{\partial\pi(\boldsymbol{x},t)}{\partial t} &= \boldsymbol{\nabla}^2\varphi(\boldsymbol{x},t)-m^2\,\varphi(\boldsymbol{x},t). \qquad (17)
\end{aligned}$$

Substituting (16) in the LHS of (17) we obtain the operator version of the Klein-Gordon equation (6),

$$\left(\Box+m^2\right)\;\varphi=0.$$

As a result, the form of the solution will also remain same as that in the classical case i.e. (8) except that now the amplitude or coefficient $\varphi(\omega_{\boldsymbol{k}},\boldsymbol{k})$ is an operator, say $\hat{\varphi}(\omega_{\boldsymbol{k}},\boldsymbol{k})$. Redefining this operator,

$$\frac{\hat{\varphi}(\omega_{\boldsymbol{k}},\boldsymbol{k})}{\sqrt{(2\pi)^5 2\omega_{\boldsymbol{k}}}}\rightarrow a(\boldsymbol{k}),$$

we have the following standard form of the Klein-Gordon quantum field operator,

$$\varphi(x)=\int\frac{d^3\boldsymbol{k}}{\sqrt{(2\pi)^3\,2\omega_{\boldsymbol{k}}}}\left(a(\boldsymbol{k})\;e^{-ik.x}+a^\dagger(\boldsymbol{k})\;e^{ik.x}\right). \qquad (18)$$

The point of this redefining the operator $\varphi(\omega_{\boldsymbol{k}}, \boldsymbol{k})$ in terms of $a(\boldsymbol{k})$ will become clear shortly. In some texts, one can find an alternative form,

$$\varphi(x) = \int d^3\boldsymbol{k}\ \left(a(\boldsymbol{k})\ f_{\boldsymbol{k}}(x) + \text{h.c.}\right), \qquad f_{\boldsymbol{k}}(x) = \frac{e^{-ik.x}}{\sqrt{(2\pi)^3\, 2\omega_{\boldsymbol{k}}}}, \tag{19}$$

where h.c. stands for "hermitian conjugate". The conjugate momentum operator can then be obtained,

$$\pi(x) = \dot{\varphi}(x) = \int \frac{d^3\boldsymbol{k}}{\sqrt{(2\pi)^3\, 2\omega_{\boldsymbol{k}}}} \left(-i\omega_{\boldsymbol{k}}\ a(\boldsymbol{k})\ e^{-ik.x} + \text{h.c.}\right) = \int d^3\boldsymbol{k}\ \left(-i\omega_{\boldsymbol{k}}\ a(\boldsymbol{k})\ f_{\boldsymbol{k}}(x) + \text{h.c.}\right). \tag{20}$$

N.B.: In the antiquated and incorrect way of thinking about the Klein-Gordon field, $\varphi(x)$, as single particle quantum mechanical wave function for a free relativistic point particle, the mode functions $f_k(x)$ are regarded as the momentum eigenstate wave-functions,

$$f_{\boldsymbol{k}}(x) = \langle \boldsymbol{x} \big| \boldsymbol{k}(t) \rangle$$

which obey the orthonormality conditions wrt to the "Klein-Gordon" norm

$$(f_{\boldsymbol{k}}, f_{\boldsymbol{k}'}) \equiv \int d^3\boldsymbol{x} f^*_{\boldsymbol{k}}(x)\ i \overleftrightarrow{\partial}_0\ f_{\boldsymbol{k}'}(x) = \delta^3\left(\boldsymbol{k} - \boldsymbol{k}'\right), \tag{21}$$

and,

$$(f^*_{\boldsymbol{k}}, f_{\boldsymbol{k}'}) \equiv \int d^3\boldsymbol{x} f_{\boldsymbol{k}}(x)\ i \overleftrightarrow{\partial}_0\ f_{\boldsymbol{k}'}(x) = 0.$$

Here $\overleftrightarrow{\partial}_0$ is defined as $a \overleftrightarrow{\partial}_0 b = a\partial_0 b - b\partial_0 a$.

The operators $a(\boldsymbol{k})$ and $a^\dagger(\boldsymbol{k})$ are going to play a major role in what is to follow from here on about the Hilbert space of states of the free scalar field theory. From the ETCCR's (1413) it follows that the operators $a_{\boldsymbol{k}}$ and $a^\dagger_{\boldsymbol{k}'}$ obey the following commutation relations,

$$\left[a(\boldsymbol{k}), a^\dagger(\boldsymbol{k}')\right] = \delta^3(\boldsymbol{k} - \boldsymbol{k}'), \tag{22}$$

$$[a(\boldsymbol{k}), a(\boldsymbol{k}')] = \left[a^\dagger(\boldsymbol{k}), a^\dagger(\boldsymbol{k}')\right] = 0. \tag{23}$$

Homework: Using the ETCCR's (14)-(13) derive the commutation relations (22)-(23) for $a_{\boldsymbol{k}}, a^\dagger_{\boldsymbol{k}'}$.
(Hint: First express $a_{\boldsymbol{k}}$ and $a^\dagger_{\boldsymbol{k}'}$ in terms of the field and its conjugate momentum, $\varphi(x), \pi(x)$. Alternatively use the orthonormality conditions (21) to express $a_{\boldsymbol{k}}, a^\dagger_{\boldsymbol{k}'}$ as Fourier coefficients of φ).

Plugging the "mode expansions" (19) & (20) of the free real scalar field and the conjugate momentum field in the expressions for the energy/Hamiltonian operator H, (9) ,and linear momentum operator $\boldsymbol{P}$, (10) we get,

$$H = \int d^3\boldsymbol{k}\ \omega_{\boldsymbol{k}}\ \frac{1}{2}\left(a(\boldsymbol{k})a^\dagger(\boldsymbol{k}) + a^\dagger(\boldsymbol{k})a(\boldsymbol{k})\right), \tag{24}$$

$$\boldsymbol{P} = \int d^3\boldsymbol{k}\ \boldsymbol{k}\ \frac{1}{2}\left(a(\boldsymbol{k})a^\dagger(\boldsymbol{k}) + a^\dagger(\boldsymbol{k})a(\boldsymbol{k})\right). \tag{25}$$

Homework: Derive (24) and (25).

2.1 The free scalar field as a collection of infinite number of independent harmonic oscillators

It is evident that the commutation relations (22) and (23) are those of an infinite set of simple harmonic creation operators, $a^\dagger(\boldsymbol{k})$ and annihilation operators, $a(\boldsymbol{k})$ labeled by the continuous index, $\boldsymbol{k}$. This can be easily seen if one goes back to the discrete label case, i.e. consider N decoupled (noninteracting) harmonic oscillators labeled by discrete index, say i or j, where $i, j \in \{1, \ldots, N\}$. The i-th harmonic oscillator is described by its creation and annihilation operators, namely $a_i^\dagger, a_i$. Their commutation relations is,

$$\left[a_i, a_j^\dagger\right] = \delta_{ij},$$

$$[a_i, a_j] = \left[a_i^\dagger, a_j^\dagger\right] = 0.$$

Now if we go from the discrete indices to continuum labels by sending $N \to \infty$ and replacing $i \to \boldsymbol{k}$, $j \to \boldsymbol{k}'$, and replacing the Kronecker delta by the Dirac delta,

$$\delta_{ij} \to \delta^3(\boldsymbol{k} - \boldsymbol{k}'),$$

then these commutation rules become same as (22) and (23), i.e. those of a free real quantum scalar in wave-vector space.

Similarly, consider the Hamiltonian of this system of N decoupled harmonic oscillators. The Hamiltonian of a single harmonic oscillator of frequency ω and creation-annihilation operators $a^\dagger, a$ is

$$h = \frac{1}{2}\omega\left(a^\dagger a + a a^\dagger\right). \tag{26}$$

So the energy of Nsuch non-interacting harmonic oscillators labeled by the discrete index i will be the sum of energy of individual oscillators:

$$H = \sum_{i=1}^{N} \frac{1}{2}\omega_i \left(a_i a_i^\dagger + a_i^\dagger a_i\right).$$

Again in the continuum version where $N \to \infty$ and the discrete label i is replaced by a continuum label $\boldsymbol{k}$, we have to replace the sum over i by the integral over $\boldsymbol{k}$, $\sum_i \to \int d^3\boldsymbol{k}$

$$H = \int d^3\boldsymbol{k}\, \frac{1}{2}\omega_{\boldsymbol{k}} \left(a(\boldsymbol{k})\, a^\dagger(\boldsymbol{k}) + a^\dagger(\boldsymbol{k})\, a(\boldsymbol{k})\right),$$

which is exactly what we have for the real scalar field Hamiltonian (24), with the continuous label $\boldsymbol{k}$ being identified with a point in wave-vector space. **Thus we have established that the free real scalar quantum field is identical to an infinite set of decoupled (noninteracting) harmonic oscillators, one located at every point in wave-vector space, $\boldsymbol{k}$.**

2.2 The Hilbert space of states: Fock space basis (occupation number basis)

Let's work out the energy eigenstates of the free real quantum scalar field. Before we do that we review some facts about the Hilbert space of states of a single harmonic oscillator with frequency ω. The energy eigenstates of this *single* harmonic oscillator are labeled by the eigenstates of the level number operator, $N \equiv a^\dagger a$ because the Hamiltonian (26) can be expressed as,

$$h = \frac{1}{2}\omega\left(a^\dagger a + a a^\dagger\right) = \frac{1}{2}\omega\left(a^\dagger a + \underbrace{\left[a, a^\dagger\right]}_{=1} + a^\dagger a\right) = \left(N + \frac{1}{2}\right)\omega.$$

Consider a state of the level number operator, say $|n\rangle$ defined by

$$N\,|n\rangle = n\,|n\rangle\,.$$

This is also an energy eigenstate and the energy eigenvalue of this state is,

$$E_n = \left(n + \frac{1}{2}\right)\omega.$$

Thus the level number n represents the energy level. From the commutation relation, $\left[N, a^\dagger\right] = a^\dagger$, one realizes that the creation operator acts on the state $|n\rangle$ and increases the level number by one unit,

$$a^\dagger\,|n\rangle = \sqrt{n+1}\,|n+1\rangle\,,$$

while the commutation relation $[N, a] = -a$ implies that the annihilation operator lowers the level number of a state by one unit,

$$a\,|n\rangle = \sqrt{n}\,|n-1\rangle\,.$$

In particular when $n = 0$, one reaches a state of lowest level number, $|0\rangle$ which is annihilated by a

$$a\,|0\rangle = 0.$$

Thus the level number n takes positive semidefinite integer values, $n = 0, 1, 2, \ldots$. Thus the energy spectrum is,

$$E_n = \left(n + \frac{1}{2}\right)\omega, \qquad n = 0, 1, 2, \ldots,$$

which bounded from below with the lowest level being of energy,

$$E_0 = \frac{1}{2}\omega.$$

The n-th energy eigenstate can be obtained by repeated applications of the n creation operators on the vacuum:

$$|n\rangle = \frac{\left(a^\dagger\right)^n}{\sqrt{n!}}|0\rangle.$$

Since the the n-th energy eigenstate has an energy $n\,\omega$ more than the vacuum state, the n-th energy level of a harmonic oscillator can be thought of as a state containing n quanta (packets of energy) with energy ω. In particular the vacuum is devoid of any quanta. In such an interpretation the level number n is also called the *occupation*

number.

Next consider the case of a finite number, say N of decoupled harmonic oscillators labeled by the discrete index, i. The Hamiltonian for this system is the sum of the Hamiltonian of the individual oscillators,

$$H = \sum_{i=1}^{N} \omega_i \left(\hat{n}_i + \frac{1}{2} \right),$$

where

$$\hat{n}_i = a_i^\dagger a_i$$

is the level number operator of the i-th oscillator. One can also define a total level number operator,

$$\hat{n} \equiv \sum_{i=1}^{N} \hat{n}_i = \sum_{i=1}^{N} a_i^\dagger a_i. \tag{27}$$

Evidently,

$$[\hat{n}_i, \hat{n}] = 0 = [\hat{n}_i, \hat{n}_j], \quad [\hat{n}_i, H] = 0$$

The ground state/ vacuum state is given by the direct product of the vacuum states of the individual oscillators,

$$\big|0\big\rangle = \big|0\big\rangle_1 \otimes \big|0\big\rangle_2 \otimes \ldots \otimes \big|0\big\rangle_N. \tag{28}$$

Evidently, the vacuum state is annihilated by either of the lowering operators,

$$a_i \big|0\big\rangle = 0, \quad \forall i = 1, \ldots, N. \tag{29}$$

The energy eigenstates of this system is given by the direct product state(s) of the form:

$$|n_1, n_2, \ldots, n_N\rangle \equiv \big|n_1\big\rangle_1 \otimes \big|n_2\big\rangle_2 \otimes \ldots \otimes \big|n_N\big\rangle_N = \frac{\left(a_1^\dagger\right)^{n_1}}{\sqrt{n_1!}} \big|0\big\rangle_1 \otimes \frac{\left(a_2^\dagger\right)^{n_2}}{\sqrt{n_2!}} \big|0\big\rangle_2 \otimes \ldots \otimes \frac{\left(a_N^\dagger\right)^{n_N}}{\sqrt{n_N!}} \big|0\big\rangle_N$$

$$\Rightarrow |n_1, n_2, \ldots, n_N\rangle = \frac{\left(a_1^\dagger\right)^{n_1}}{\sqrt{n_1!}} \frac{\left(a_2^\dagger\right)^{n_2}}{\sqrt{n_2!}} \ldots \frac{\left(a_N^\dagger\right)^{n_N}}{\sqrt{n_N!}} \big|0\big\rangle, \tag{30}$$

i.e. a state where the oscillator with label 1 is in the level n_1, the oscillator with label 2 is in the level n_2, so on. The n_i's are positive integers or zero. The total level number of this state is,

$$n = \sum_{i=1}^{N} n_i. \tag{31}$$

The energy of this state is evidently the sum of the energies of the individual oscillators,

$$E_{n_1, n_2, \ldots, n_N} = \sum_{i=1}^{N} \left(n_i + \frac{1}{2} \right) \omega_i.$$

In particular the ground state energy is,

$$E_0 = \sum_{i=1}^{N} \frac{1}{2} \omega_i.$$

We will use a condensed notation where we denote the state (30) by abstract dummy index, i

$$\big|\,\{n_i\}\big\rangle \equiv \prod_{i=1}^{N} \otimes \big|n_i\big\rangle_i.$$

In this case, the number n_i is the excitation level of the i-th oscillator and the $n = \sum_i n_i$ is the total level number. Alternatively we say there are n_i quanta present in the i-th oscillator.

Now let's go over to the continuum version by replacing the discrete label i by a continuous label $\boldsymbol{k}$, $i \to \boldsymbol{k}$. The vacuum state $\big|0\big\rangle$ is by all the lowering operators corresponding arbitrary $\boldsymbol{k}$, so analogous to (29)

$$a(\boldsymbol{k})\big|0\big\rangle = 0, \forall \boldsymbol{k},$$

The occupation number or level number of this state is obtained by acting on the vacuum by the number operator. The the total (level) number operator is obtained by replacing the discrete label i by a continuous label $\boldsymbol{k}$, $i \to \boldsymbol{k}$ in equation (27),

$$\hat{N} = \int d^3\boldsymbol{k}\, \hat{n}(\boldsymbol{k}), \quad n(\boldsymbol{k}) = a^\dagger(\boldsymbol{k})\, a(\boldsymbol{k}).$$

Clearly then, $n(\boldsymbol{k})\, d^3\boldsymbol{k}$ is now the **occupation number** of the oscillator labeled by the continuum index $\boldsymbol{k}$ with frequency $\omega_{\boldsymbol{k}}$. So $n(\boldsymbol{k})$ is now the **occupation number density (per unit volume in $\boldsymbol{k}$ space)** for the oscillators with wave-number in the range/interval $\boldsymbol{k}$ and $\boldsymbol{k} + d\boldsymbol{k}$. Acting with this on the vacuum state, we obtain

$$\hat{N}\big|0\big\rangle = \int d^3\boldsymbol{k}\, a^\dagger(\boldsymbol{k})\, \underbrace{a(\boldsymbol{k})\, \big|0\big\rangle}_{=0} = 0\, \big|0\big\rangle.$$

Thus the vacuum state is an eigenstate of the number operator with eigenvalue 0 i.e. the free quantum scalar vacuum state is devoid of any quanta (just like in the harmonic oscillator vacuum).

Next consider the "first excited states" i.e. those obtained by acting on the vacuum by a single raising operator, e.g.,

$$a^\dagger(\boldsymbol{k})\, \big|0\big\rangle,$$

for some vector $\boldsymbol{k}$. By analogy from the discrete N-oscillator case, we expect this to be a state containing a single quantum. Let's verify it by acting on this state by the occupation number operator,

$$\begin{aligned}
\hat{N}\, a^\dagger(\boldsymbol{k})\, \big|0\big\rangle &= \int d^3\boldsymbol{q}\, a^\dagger(\boldsymbol{q})\, \underline{a(\boldsymbol{q})\, a^\dagger(\boldsymbol{k})}\, \big|0\big\rangle \\
&= \int d^3\boldsymbol{q}\, a^\dagger(\boldsymbol{q})\, \Big(\big[a(\boldsymbol{q}), a^\dagger(\boldsymbol{k})\big] + a^\dagger(\boldsymbol{k})\, a(\boldsymbol{q})\Big)\, \big|0\big\rangle \\
&= \int d^3\boldsymbol{q}\, a^\dagger(\boldsymbol{q})\, \Big(\delta^3\left(\boldsymbol{q} - \boldsymbol{k}\right) + a^\dagger(\boldsymbol{k})\, a(\boldsymbol{q})\Big)\, \big|0\big\rangle \\
&= a^\dagger(\boldsymbol{k})\, \big|0\big\rangle \\
&= 1\, a^\dagger(\boldsymbol{k})\, \big|0\big\rangle.
\end{aligned} \tag{32}$$

Thus we have checked that the state $a^\dagger(\boldsymbol{k})\,\big|0\rangle$ is an eigenstate of the occupation number operator with eigenvalue 1, i.e. a single quantum state.

Then the higher states are then obtained by acting repeatedly with the raising or creation operators for many different $\boldsymbol{k}$'s on this vacuum state analogous to the state (30).,

$$\big|n_i(\boldsymbol{k}_1), n_2(\boldsymbol{k}_2), \ldots, n_l(\boldsymbol{k}_l)\rangle \equiv \frac{\big(a^\dagger(\boldsymbol{k}_1)\big)^{n_1}}{\sqrt{n_1!}} \frac{\big(a^\dagger(\boldsymbol{k}_1)\big)^{n_1}}{\sqrt{n_1!}} \ldots \frac{\big(a^\dagger(\boldsymbol{k}_N)\big)^{n_l}}{\sqrt{n_N!}} \big|0\rangle. \tag{33}$$

This state has the oscillator with wave-number $\boldsymbol{k}_1$ excited to level n_1, the oscillator with wave-number $\boldsymbol{k}_2$ excited to level n_1 and so on and so forth. Alternatively in this state one has n_1 quanta with wavenumber $\boldsymbol{k}_1$, n_2 quanta of wavenumber $\boldsymbol{k}_2$ etc. This can be easily verified by acting on state (33) by the number density operator,

$$\begin{aligned}
\hat{n}(\boldsymbol{k})\,\big|n_i(\boldsymbol{k}_1), n_2(\boldsymbol{k}_2), \ldots, n_l(\boldsymbol{k}_l)\rangle &= a^\dagger(\boldsymbol{k})\,a(\boldsymbol{k})\,\frac{\big(a^\dagger(\boldsymbol{k}_1)\big)^{n_1}}{\sqrt{n_1!}} \frac{\big(a^\dagger(\boldsymbol{k}_1)\big)^{n_1}}{\sqrt{n_1!}} \ldots \frac{\big(a^\dagger(\boldsymbol{k}_l)\big)^{n_l}}{\sqrt{n_l!}} \big|0\rangle \\
&= a^\dagger(\boldsymbol{k})\,\left(\left[a(\boldsymbol{k}), \frac{\big(a^\dagger(\boldsymbol{k}_1)\big)^{n_1}}{\sqrt{n_1!}} \frac{\big(a^\dagger(\boldsymbol{k}_1)\big)^{n_1}}{\sqrt{n_1!}} \ldots \frac{\big(a^\dagger(\boldsymbol{k}_l)\big)^{n_l}}{\sqrt{n_l!}}\right] + \frac{\big(a^\dagger(\boldsymbol{k}_1)\big)^{n_1}}{\sqrt{n_1!}} \frac{\big(a^\dagger(\boldsymbol{k}_1)\big)^{n}}{\sqrt{n_1!}}\right. \\
&= a^\dagger(\boldsymbol{k})\,\left[a(\boldsymbol{k}), \frac{\big(a^\dagger(\boldsymbol{k}_1)\big)^{n_1}}{\sqrt{n_1!}} \frac{\big(a^\dagger(\boldsymbol{k}_1)\big)^{n_1}}{\sqrt{n_1!}} \ldots \frac{\big(a^\dagger(\boldsymbol{k}_l)\big)^{n_l}}{\sqrt{n_l!}}\right] \big|0\rangle \qquad (\text{since } a(\boldsymbol{k})\big|0\rangle = \\
&= \sum_{i=1}^{l} a^\dagger(\boldsymbol{k})\,\frac{\big(a^\dagger(\boldsymbol{k}_1)\big)^{n_1}}{\sqrt{n_1!}} \frac{\big(a^\dagger(\boldsymbol{k}_1)\big)^{n_1}}{\sqrt{n_1!}} \ldots \left[a(\boldsymbol{k}), \frac{\big(a^\dagger(\boldsymbol{k}_i)\big)^{n_i}}{\sqrt{n_i!}}\right] \ldots \big| \frac{\big(a^\dagger(\boldsymbol{k}_l)\big)^{n_l}}{\sqrt{n_l!}} \big|0\rangle \\
&= \sum_{i=1}^{l} a^\dagger(\boldsymbol{k})\,\frac{\big(a^\dagger(\boldsymbol{k}_1)\big)^{n_1}}{\sqrt{n_1!}} \frac{\big(a^\dagger(\boldsymbol{k}_1)\big)^{n_1}}{\sqrt{n_1!}} \ldots n_i \frac{\big(a^\dagger(\boldsymbol{k}_i)\big)^{n_i-1}}{\sqrt{n_i!}} \big[a(\boldsymbol{k}), a^\dagger(\boldsymbol{k}_i)\big] \ldots \frac{\big(a^\dagger(\boldsymbol{k}_l)\big)}{\sqrt{n_l!}} \\
&= \sum_{i=1}^{l} a^\dagger(\boldsymbol{k})\,\frac{\big(a^\dagger(\boldsymbol{k}_1)\big)^{n_1}}{\sqrt{n_1!}} \frac{\big(a^\dagger(\boldsymbol{k}_1)\big)^{n_1}}{\sqrt{n_1!}} \ldots n_i \frac{\big(a^\dagger(\boldsymbol{k}_i)\big)^{n_i-1}}{\sqrt{n_i!}} \delta^3(\boldsymbol{k}-\boldsymbol{k}_i) \ldots \frac{\big(a^\dagger(\boldsymbol{k}_l)\big)^{n_l}}{\sqrt{n_l!}} \big|0 \\
&= \sum_{i=1}^{l} n_i\,\delta^3(\boldsymbol{k}-\boldsymbol{k}_i)\,\frac{\big(a^\dagger(\boldsymbol{k}_1)\big)^{n_1}}{\sqrt{n_1!}} \frac{\big(a^\dagger(\boldsymbol{k}_1)\big)^{n_1}}{\sqrt{n_1!}} \ldots \frac{\big(a^\dagger(\boldsymbol{k}_i)\big)^{n_i}}{\sqrt{n_i!}} \ldots \frac{\big(a^\dagger(\boldsymbol{k}_l)\big)^{n_l}}{\sqrt{n_l!}} \big|0\rangle \\
&= \left(\sum_{i=1}^{l} n_i\,\delta^3(\boldsymbol{k}-\boldsymbol{k}_i)\right)\,\big|n_i(\boldsymbol{k}_1), n_2(\boldsymbol{k}_2), \ldots, n_l(\boldsymbol{k}_l)\rangle
\end{aligned}$$

So this is an eigenstate of the number density operator, with eigenvalue $n = \sum_{i=1}^{l} n_i\,\delta^3(\boldsymbol{k}-\boldsymbol{k}_i)$, which is clearly a density (recall from electrostatics the density of a configuration of point charges is given by a sum of Dirac delta functions). Further this state is also an eigenstate of the total occupation number operator, $\hat{N} = \int d^3\boldsymbol{k}\,\hat{n}(\boldsymbol{k}),\ n(\boldsymbol{k}) = a^\dagger(\boldsymbol{k})\,a(\boldsymbol{k})$,

$$\begin{aligned}
\hat{N}\,\big|n_i(\boldsymbol{k}_1), n_2(\boldsymbol{k}_2), \ldots n_i(\boldsymbol{k}_i), \ldots n_l(\boldsymbol{k}_l)\rangle &= \int d^3\boldsymbol{k}\,\hat{n}(\boldsymbol{k})\,\big|n_i(\boldsymbol{k}_1), n_2(\boldsymbol{k}_2), \ldots n_i(\boldsymbol{k}_i), \ldots n_l(\boldsymbol{k}_l)\rangle \\
&= \int d^3\boldsymbol{k}\,\left(\sum_{i=1}^{l} n_i\,\delta^3(\boldsymbol{k}-\boldsymbol{k}_i)\right)\,\big|n_i(\boldsymbol{k}_1), n_2(\boldsymbol{k}_2), \ldots n_i(\boldsymbol{k}_i), \ldots n_l(\boldsymbol{k}_l)\rangle \\
&= N\,\big|n_i(\boldsymbol{k}_1), n_2(\boldsymbol{k}_2), \ldots n_i(\boldsymbol{k}_i), \ldots n_l(\boldsymbol{k}_l)
\end{aligned}$$

where

$$N = \sum_{i=1}^{l} n_i$$

is total number level number of all the oscillators excited. Thus this is a state containing a total of N quanta, out of which n_1 quanta are of type $\boldsymbol{k}_1$, n_2 quanta are of type $\boldsymbol{k}_2$ etc.

2.3 The particle (quanta) interpretation

In this section we show that the states (33) actually represent a state of N noninteracting point particles of mass m out of which n_1 of them have with linear momentum $\boldsymbol{k}_1$, n_2 of them have with linear momentum $\boldsymbol{k}_2$, and so on and so forth. For this purpose we will need to recall the Hamiltonian expressed as a mode expansion (24)

$$H = \int d^3\boldsymbol{k}\, \frac{1}{2}\omega_{\boldsymbol{k}} \left(a^\dagger(\boldsymbol{k})\, a(\boldsymbol{k}) + a(\boldsymbol{k})\, a^\dagger(\boldsymbol{k})\right). \tag{34}$$

and the linear momentum operator expressed as a mode expansion,

$$\boldsymbol{P} = \int d^3\boldsymbol{k}\, \frac{1}{2}\, \boldsymbol{k}\, \left(a^\dagger(\boldsymbol{k})\, a(\boldsymbol{k}) + a(\boldsymbol{k})\, a^\dagger(\boldsymbol{k})\right)$$

Here $n(\boldsymbol{k})$ is now the **level number density** of the oscillator labeled by the continuum index $\boldsymbol{k}$ with frequency $\omega_{\boldsymbol{k}}$. The reason $n(\boldsymbol{k})$ is a density is because it is being integrated over $d^3\boldsymbol{k}$, i.e. the level number is $n(\boldsymbol{k})\, d^3\boldsymbol{k}$. For the case of the free scalar quantum field theory, the continuum index $\boldsymbol{k}$ is the wave-vector and the frequency is $\omega_{\boldsymbol{k}} = \sqrt{\boldsymbol{k}^2 + m^2}$. **In this case, $n(\boldsymbol{k})$ is interpreted as the *number density of particles* of mass m and linear momentum $\boldsymbol{k}$, or equivalently $n(\boldsymbol{k})\, d^3\boldsymbol{k}$ is the number of particles of mass m and linear momentum $\boldsymbol{k}$.** This is easily demonstrated as follows. Consider first vacuum state, $\big|0\big\rangle$. This is an eigenstate of the energy and momentum operators, as can be seen by acting with the energy and linear momentum operators on it. First consider the energy operator, H

$$H\,\big|0\big\rangle = \int d^3\boldsymbol{k}\, \frac{1}{2}\omega_{\boldsymbol{k}} \left(a^\dagger(\boldsymbol{k})\, a(\boldsymbol{k}) + a(\boldsymbol{k})\, a^\dagger(\boldsymbol{k})\right)\, \big|0\big\rangle = E_0\,\big|0\big\rangle$$

where E_0 is the vacuum energy[1]

$$E_0 = \int d^3\boldsymbol{k}\, \frac{1}{2}\omega_{\boldsymbol{k}}\, \delta^3(\boldsymbol{0}),$$

and,

$$\boldsymbol{P}\,\big|0\big\rangle = \int d^3\boldsymbol{k}\, \frac{1}{2}\, \boldsymbol{k}\, \left(a^\dagger(\boldsymbol{k})\, a(\boldsymbol{k}) + a(\boldsymbol{k})\, a^\dagger(\boldsymbol{k})\right)\, \big|0\big\rangle = \left(\int d^3\boldsymbol{k}\, \boldsymbol{k}\, \frac{1}{2}\right)\, \delta^3(0) = 0\,\big|0\big\rangle,$$

as the $\boldsymbol{k}$-integrand is an odd function and the range is over $(-\infty, \infty)$. Thus the vacuum state is a simultaneous eigenstate of the occupation number operator, the Hamiltonian operator and the linear momentum operator with eigenvalues $0, E_0, \boldsymbol{0}$ respectively.

[1] More discussion on the divergent vaccum energy in Sec. 3

Next consider the state:

$$\big|\Psi\rangle = a^\dagger(\boldsymbol{p})\big|0\rangle$$

This state has a single quantum as shown in (32),

$$N\ \big|\Psi\rangle = 1\ \big|\Psi\rangle.$$

This is also an energy eigenstate and the energy eigenvalue can be obtained by acting with the H operator in this state,

$$\begin{aligned} H\ \big|\Psi\rangle &= \int d^3\boldsymbol{k}\ \frac{1}{2}\omega_{\boldsymbol{k}}\left(a^\dagger(\boldsymbol{k})\,a(\boldsymbol{k}) + a(\boldsymbol{k})\,a^\dagger(\boldsymbol{k})\right)\ a^\dagger(\boldsymbol{p})\big|0\rangle \\ &= \int d^3\boldsymbol{k}\ \frac{1}{2}\omega_{\boldsymbol{k}}\left(a^\dagger(\boldsymbol{k})\,a(\boldsymbol{k})\,a^\dagger(\boldsymbol{p})\big|0\rangle + a(\boldsymbol{k})\,a^\dagger(\boldsymbol{k})\,a^\dagger(\boldsymbol{p})\big|0\rangle\right) \\ &= (\omega_{\boldsymbol{p}} + E_0)\ \big|\Psi\rangle. \end{aligned}$$

Here we have use the algebraic simplifications,

$$\begin{aligned} a^\dagger(\boldsymbol{k})\,a(\boldsymbol{k})\,a^\dagger(\boldsymbol{p})\big|0\rangle &= a^\dagger(\boldsymbol{k})\ \big[a(\boldsymbol{k}), a^\dagger(\boldsymbol{p})\big]\ \big|0\rangle + a^\dagger(\boldsymbol{k})\,a^\dagger(\boldsymbol{p})\ \cancel{a(\boldsymbol{k})\big|0\rangle} \\ &= a^\dagger(\boldsymbol{k})\,\delta^3(\boldsymbol{k}-\boldsymbol{p})\big|0\rangle, \end{aligned} \tag{35}$$

and

$$\begin{aligned} \underline{a(\boldsymbol{k})\,a^\dagger(\boldsymbol{k})}\,a^\dagger(\boldsymbol{p})\big|0\rangle &= \big[a(\boldsymbol{k}), a^\dagger(\boldsymbol{k})\big]\ a^\dagger(\boldsymbol{p})\big|0\rangle + a^\dagger(\boldsymbol{k})\,\underline{a(\boldsymbol{k})\,a^\dagger(\boldsymbol{p})}\big|0\rangle \\ &= \big[a(\boldsymbol{k}), a^\dagger(\boldsymbol{k})\big]\ a^\dagger(\boldsymbol{p})\big|0\rangle + a^\dagger(\boldsymbol{k})\ \big[a(\boldsymbol{k}), a^\dagger(\boldsymbol{p})\big]\ \big|0\rangle + a^\dagger(\boldsymbol{k})\,a^\dagger(\boldsymbol{p})\,\cancel{a(\boldsymbol{k})\big|0\rangle} \\ &= \delta^3(\boldsymbol{0})\,a^\dagger(\boldsymbol{p})\big|0\rangle + a^\dagger(\boldsymbol{k})\,\delta^3(\boldsymbol{k}-\boldsymbol{p})\big|0\rangle, \end{aligned} \tag{36}$$

to arrive at this result,

$$\begin{aligned} H\ \big|\Psi\rangle &= \int d^3\boldsymbol{k}\,\omega_{\boldsymbol{k}}\left(\delta^3(\boldsymbol{k}-\boldsymbol{p}) + \frac{1}{2}\right)\ \big|\Psi\rangle \\ &= (\omega_{\boldsymbol{p}} + E_0)\ \big|\Psi\rangle. \end{aligned}$$

Thus the energy of this state is $\omega_{\boldsymbol{p}} = \sqrt{\boldsymbol{p}^2 + m^2}$ above the vacuum:

$$E_\psi - E_0 = \omega_{\boldsymbol{p}}.$$

The linear momentum of the state is obtained by acting on this state with the $\boldsymbol{P}$ and using the simplifications (35), (36)

$$\begin{aligned} \boldsymbol{P}\ \big|\Psi\rangle &= \int d^3\boldsymbol{k}\ \frac{1}{2}\boldsymbol{k}\left(a^\dagger(\boldsymbol{k})\,a(\boldsymbol{k}) + a(\boldsymbol{k})\,a^\dagger(\boldsymbol{k})\right)\ a^\dagger(\boldsymbol{p})\big|0\rangle \\ &= \int d^3\boldsymbol{k}\ \frac{1}{2}\boldsymbol{k}\left(2\,a^\dagger(\boldsymbol{k})\,\delta^3(\boldsymbol{k}-\boldsymbol{p}) + \delta^3(\boldsymbol{0})\,a^\dagger(\boldsymbol{p})\right)\ \big|0\rangle \\ &= \boldsymbol{p}\,a^\dagger(\boldsymbol{p})\big|0\rangle \\ &= \boldsymbol{p}\ \big|\psi\rangle. \end{aligned}$$

As expected this is a momentum eigenstate with eigenvalue $\boldsymbol{p}$.

2.3.1 Particle interpretation

Since this state $a^\dagger(\boldsymbol{p})|0\rangle$ represents an excitation with energy $E = \sqrt{\boldsymbol{p}^2 + m^2}$ and momentum $\boldsymbol{p}$, it can be identified with a single particle of mass m and linear momentum $\boldsymbol{p}$. Similarly one can show that the state $\left(a^\dagger(\boldsymbol{p})\right)^n |0\rangle$ creates an excitation which has energy, nE and momentum $n\boldsymbol{p}$, i.e. this state can be identified with a state containing n free particles of mass m and linear momentum $\boldsymbol{p}$. More generally, the state

$$\left(a^\dagger(\boldsymbol{p}_1)\right)^{n_1} \left(a^\dagger(\boldsymbol{p}_2)\right)^{n_2} \ldots \left(a^\dagger(\boldsymbol{p}_N)\right)^{n_N} |0\rangle$$

represents an excitation of energy,

$$E = n_1\sqrt{\boldsymbol{p}_1^2 + m^2} + n_2\sqrt{\boldsymbol{p}_2^2 + m^2} + \ldots + n_N\sqrt{\boldsymbol{p}_N^2 + m^2}$$

and momentum,

$$\boldsymbol{P} = n_1\boldsymbol{p}_1 + n_2\boldsymbol{p}_2 + \ldots + n_N\boldsymbol{p}_N.$$

Thus it can be identified with a state of n_1 free particles of mass m and momentum $\boldsymbol{p}_1$, n_2 free particles of mass m and momentum $\boldsymbol{p}_2$, etc.

Homework: Prove the last statement.

The occupation number operator can then be interpreted as **particle number operator**.

3 Vacuum energy of the free scalar quantum field: UV and IR divergences

The Hamiltonian of the free quantum scalar field is,

$$\begin{aligned} H &= \int d^3\boldsymbol{k}\ \frac{1}{2}\omega_{\boldsymbol{k}}\ \left(a^\dagger(\boldsymbol{k})a(\boldsymbol{k}) + a(\boldsymbol{k})a^\dagger(\boldsymbol{k})\right) \\ &= \int d^3\boldsymbol{k}\ \frac{1}{2}\omega_{\boldsymbol{k}}\ \left(2a^\dagger(\boldsymbol{k})a(\boldsymbol{k}) + \left[a(\boldsymbol{k}), a^\dagger(\boldsymbol{k})\right]\right) \\ &= \int d^3\boldsymbol{k}\ \omega_{\boldsymbol{k}}\ \left(a^\dagger(\boldsymbol{k})a(\boldsymbol{k}) + \frac{1}{2}\delta^3(\boldsymbol{0})\right). \end{aligned}$$

The vacuum is an eigenstate of the Hamiltonian with the eigenvalue,

$$\begin{aligned} E_0 = \langle 0|H|0\rangle &= \int d^3\boldsymbol{k}\ \omega_{\boldsymbol{k}}\ \left(\cancelto{0}{\langle 0|a^\dagger(\boldsymbol{k})a(\boldsymbol{k})|0\rangle} + \langle 0|\frac{1}{2}\delta^3(\boldsymbol{0})|0\rangle\right) \\ &= \delta^3(\boldsymbol{0})\left(\int d^3\boldsymbol{k}\ \frac{1}{2}\omega_{\boldsymbol{k}}\right). \end{aligned}$$

Thus the vacuum energy is divergent on two accounts. First we have the divergent integral, $\int d^3\boldsymbol{k}\ \frac{1}{2}\omega_{\boldsymbol{k}}$, which represents the sum total of ground state energy of oscillators of frequency $\omega_{\boldsymbol{k}}$. Since the ground state energy of a single harmonic oscillator is finite and increasing function of $|\boldsymbol{k}|$,

this energy of oscillators with large $|\boldsymbol{k}|$ will diverge. This integral diverges at large wave-numbers, i.e. when $k = |\boldsymbol{k}| \to \infty$ as,

$$\int d^3\boldsymbol{k}\ \frac{1}{2}\omega_{\boldsymbol{k}} \sim \int^{\infty} dk\ k^3 \sim k^4$$

because $d^3\boldsymbol{k} \sim k^2 dk$ while $\omega_{\boldsymbol{k}} \sim k$ at large k. This quartic divergence as $k \to \infty$ is an example of a UV divergence (ultraviolet divergence) because it stems from large k and since $k = \frac{2\pi}{\lambda}$, it means small λ or, ***short wavelengths*** i.e. the ultraviolet end of the spectrum.

On the other hand the divergence arising from the Dirac delta function in $\boldsymbol{k}$-space,

$$\delta^3(\boldsymbol{0})$$

has nothing to do with large k, but instead has to do with $\boldsymbol{k} \to 0$ i.e. ***infinitely long wavelengths*** and thus represents an Infrared divergence (IR divergence). What is the origin of this IR divergence? It can be shown that the origin of this divergence is due to the fact that in the interval $|\boldsymbol{k}|$ and $|\boldsymbol{k} + d\boldsymbol{k}|$ contains an *infinite* number of modes. Let $\Omega(\boldsymbol{k})\, d\boldsymbol{k}$ represent the number of modes in the infinitesimal interval $|\boldsymbol{k}|$ and $|\boldsymbol{k} + d\boldsymbol{k}|$. Then one can show that in the limit of infinite volume in physical space, $V = \int d^3\boldsymbol{x}$, the density of states in k-space diverges,

$$\lim_{V\to\infty} \Omega(\boldsymbol{k}) \to \infty.$$

To see this we start not from infinite space i.e. $\mathbb{R}^3$ but instead a finite dimensional box with edges L_1, L_2, L_3 with periodic boundary conditions in all three directions[2], and finally we will take the limit $V = L_1L_2L_3 \to \infty$. In such a finite dimensional box the oscillator modes (wave-vectors) are discretized instead of being continuous,

$$\boldsymbol{k} = n_1\frac{2\pi}{L_1}\hat{\boldsymbol{x}} + n_2\frac{2\pi}{L_2}\hat{\boldsymbol{y}} + n_3\frac{2\pi}{L_3}\hat{\boldsymbol{z}},$$

for three integers n_1, n_2, n_3. Now the number of states in the range $|\boldsymbol{k}|$ and $|\boldsymbol{k} + d\boldsymbol{k}|$ is then given by the number of such discrete points which lie inside a spherical shell of radius $|\boldsymbol{k}|$ and thickness $d\,|\boldsymbol{k}|$. Now each point is characterized by 3 integers and the unit cell volume for such discrete points is, $\frac{(2\pi)^3}{L_1L_2L_3}$ i.e.within this volume in $\boldsymbol{k}$-space there exist just one allowed point i.e. wave-vector . Then the number of points in the spherical shell is,

$$\Omega(\boldsymbol{k})\, d\boldsymbol{k} = \frac{4\pi\ |\boldsymbol{k}|^2\ d\,|\boldsymbol{k}|}{\left(\frac{(2\pi)^3}{L_1L_2L_3}\right)} \sim V\,|\boldsymbol{k}|^2\ d\,|\boldsymbol{k}|\,.$$

Clearly this diverges when $V \to \infty$. Such divergences arise strictly in the large volumes (large system-size) limit, and such IR divergence can be cured by putting the field theory in a very large but finite box. Then the vacuum energy becomes finite (the UV divergence can also be tamed) and is an observable/measurable quantity known as the Casimir energy (it produces a famous effect, in fact a force known as Casimir force).
at

How should we deal with the infinite vacuum energy of the free scalar field? One way to deal with this problem is realizing that the vacuum energy is not a measurable quantity and

[2]This means we are considering space with the topology of a three torus, $T^3 = S^1 \times S^1 \times S^1$ instead of $\mathbb{R}^3$.

in experiments we only measure changes in the energy level when the system makes transitions (jumps) from one energy level to another. Since all the energy levels of the free quantum scalar field has identical divergent contribution, say E_0

$$E_n = E'_n + E_0,$$

the energy differences are rendered finite!

$$E_m - E_n = E'_m + \cancel{E_0} - E'_n - \cancel{E_0} = E'_m - E'_n.$$

Here E'_n, E'_m are the finite parts. For the generic state (33),

$$E = \sum_{i=1}^{l} n_i \, \omega_{\boldsymbol{k}_i} + E_0.$$

3.1 Prescription to avoid vaccum energy: Normal ordering the Hamiltonian

The way we get around this divergence in the vacuum energy, sometimes referred to as the ***zero point energy*** is by using a particular ordering of creation and annihilation operators known as ***Normal ordering***. Normal ordering prescription is defined by the rule that any product of arbitrary number of creation and annihilation operators in an arbitrary sequence must be ordered such that ***all the creation operators are to the left and all the annihilation operators are to the right*** by using commutation rules and dropping the purely c-number pieces. We will denote the normal ordered version of a given operator $\mathcal{O}$ by the punctuation mark colon - from left and right,

$$: \mathcal{O} :$$

For example, the operator $a(\boldsymbol{k})a^\dagger(\boldsymbol{p})$ is not normal ordered because the creation operator is to the right of the annihilation operator. So we change the order by using oscillator commutator algebra,

$$\begin{aligned} a(\boldsymbol{k})a^\dagger(\boldsymbol{p}) &= \underbrace{\big[a(\boldsymbol{k}), a^\dagger(\boldsymbol{p})\big]}_{\delta^3(\boldsymbol{k}-\boldsymbol{p})} + a^\dagger(\boldsymbol{p})a(\boldsymbol{k}) \\ &= \delta^3(\boldsymbol{k}-\boldsymbol{p}) + a^\dagger(\boldsymbol{p})a(\boldsymbol{k}). \end{aligned}$$

Next we will drop the c-number piece, $\delta^3(\boldsymbol{k}-\boldsymbol{p})$ to get the normal ordered operator,

$$: a(\boldsymbol{k})a^\dagger(\boldsymbol{p}) : = a^\dagger(\boldsymbol{p})a(\boldsymbol{k}).$$

On the other hand, the operators,$a^\dagger(\boldsymbol{p})a^\dagger(\boldsymbol{k})$, or $a(\boldsymbol{p})\, a(\boldsymbol{k})$ are already normal ordered,

$$\begin{aligned} : a^\dagger(\boldsymbol{k})a^\dagger(\boldsymbol{p}) : &= a^\dagger(\boldsymbol{k})a^\dagger(\boldsymbol{p}), \\ : a(\boldsymbol{p})\, a(\boldsymbol{k}) : &= a(\boldsymbol{p})\, a(\boldsymbol{k}). \end{aligned}$$

Next, consider the operator

$$\mathcal{O} \equiv a(\boldsymbol{k}_1)\, a(\boldsymbol{k}_2)\, a^\dagger(\boldsymbol{k}_3).$$

The normal ordered version of this operator is,

$$:\mathcal{O}:=a^\dagger(\boldsymbol{k}_3)\;a(\boldsymbol{k}_1)\;a(\boldsymbol{k}_2).$$

To see how the operators $\mathcal{O}$ and $:\mathcal{O}:$ are different, we will use commutation rules between $a, a^\dagger$ to switch their orders in $\mathcal{O}$ as follows. First we switch the orders of the last two operators so that the annihilation operator $a(\boldsymbol{k}_3)$ is to the right,

$$\begin{aligned}\mathcal{O}&=a(\boldsymbol{k}_1)\;a(\boldsymbol{k}_2)\;a^\dagger(\boldsymbol{k}_3)\\&=a(\boldsymbol{k}_1)\left(\left[a(\boldsymbol{k}_2),a^\dagger(\boldsymbol{k}_3)\right]+a^\dagger(\boldsymbol{k}_3)\;a(\boldsymbol{k}_2)\right)\\&=a(\boldsymbol{k}_1)\left(\delta^3\left(\boldsymbol{k}_2-\boldsymbol{k}_3\right)+a^\dagger(\boldsymbol{k}_3)\;a(\boldsymbol{k}_2)\right)\\&=a(\boldsymbol{k}_1)\;\delta^3\left(\boldsymbol{k}_2-\boldsymbol{k}_3\right)+a(\boldsymbol{k}_1)\;a^\dagger(\boldsymbol{k}_3)\;a(\boldsymbol{k}_2).\end{aligned}$$

Next we normal order the second term by using commutation rules to place $a(\boldsymbol{k}_1)$ to the right

$$\begin{aligned}\mathcal{O}&=a(\boldsymbol{k}_1)\;\delta^3\left(\boldsymbol{k}_2-\boldsymbol{k}_3\right)+a(\boldsymbol{k}_1)\;a^\dagger(\boldsymbol{k}_3)\;a(\boldsymbol{k}_2)\\&=a(\boldsymbol{k}_1)\;\delta^3\left(\boldsymbol{k}_2-\boldsymbol{k}_3\right)+\left(\left[a(\boldsymbol{k}_1),a^\dagger(\boldsymbol{k}_3)\right]+a^\dagger(\boldsymbol{k}_3)\;a(\boldsymbol{k}_1)\right)\;a(\boldsymbol{k}_2)\\&=a(\boldsymbol{k}_1)\;\delta^3\left(\boldsymbol{k}_2-\boldsymbol{k}_3\right)+\delta^3\left(\boldsymbol{k}_1-\boldsymbol{k}_3\right)\;a(\boldsymbol{k}_2)+a^\dagger(\boldsymbol{k}_3)\;a(\boldsymbol{k}_1)\;a(\boldsymbol{k}_2)\\&=a(\boldsymbol{k}_1)\;\delta^3\left(\boldsymbol{k}_2-\boldsymbol{k}_3\right)+\delta^3\left(\boldsymbol{k}_1-\boldsymbol{k}_3\right)\;a(\boldsymbol{k}_2)+:\mathcal{O}:\end{aligned}$$

Thus we see that the difference between $\mathcal{O}$ and its normal ordered version is,

$$\mathcal{O}-:\mathcal{O}:\;\;=a(\boldsymbol{k}_1)\;\delta^3\left(\boldsymbol{k}_2-\boldsymbol{k}_3\right)+\delta^3\left(\boldsymbol{k}_1-\boldsymbol{k}_3\right)\;a(\boldsymbol{k}_2).$$

In this case this difference is not a big deal because both have the same vacuum expectation value,

$$\begin{aligned}\langle 0|\mathcal{O}|0\rangle-\langle 0|:\mathcal{O}:|0\rangle&=\underbrace{\langle 0|a(\boldsymbol{k}_1)|0\rangle}_{=0}\;\delta^3\left(\boldsymbol{k}_2-\boldsymbol{k}_3\right)+\delta^3\left(\boldsymbol{k}_1-\boldsymbol{k}_3\right)\;\underbrace{\langle 0|a(\boldsymbol{k}_2)|0\rangle}_{=0}\\&=0.\end{aligned}$$

However in general,

$$\langle 0|\mathcal{O}|0\rangle\neq\langle 0|:\mathcal{O}:|0\rangle$$

and only the **normal ordered operator has vanishing vacuum expectation value**[3],

$$\langle 0|:\mathcal{O}:|0\rangle=0$$

[3]It is tempting to claim that a normal ordered operator annihilate the vacuum while the non-normal ordered operator might not,

$$\mathcal{O}|0\rangle\neq 0=:\mathcal{O}:|0\rangle.$$

This is almost always true but not universally true. For example, consider the operator, $\mathcal{O}=a^\dagger(\boldsymbol{k})\,a^\dagger(\boldsymbol{p})$. This is already normal ordered, i.e. $\mathcal{O}=:\mathcal{O}:$, but it does not annihilate the vacuum,

$$:\mathcal{O}:|0\rangle\neq 0.$$

However the vacuum expectation value definitely vanishes,

$$\langle 0|:\mathcal{O}:|0\rangle=\langle 0|\mathcal{O}|0\rangle=\langle 0|a^\dagger(\boldsymbol{k})\,a^\dagger(\boldsymbol{p})|0\rangle=0$$

because,

$$\langle 0|a^\dagger(\boldsymbol{k})=\left(a(\boldsymbol{k})|0\rangle\right)^\dagger=0.$$

because on the right the annihilation operators destroy the vacuum i.e. $a|0\rangle = 0$, as well as on the left the creation operators kill the vacuum,

$$\langle 0|a^\dagger = \big(a|0\rangle\big)^\dagger = 0.$$

Using the normal ordering prescription for the Hamiltonian operator (24),

$$\begin{aligned} :H: &= \int d^3\boldsymbol{k}\, \frac{1}{2}\omega_{\boldsymbol{k}} \left(: a^\dagger(\boldsymbol{k})\, a(\boldsymbol{k}) : + : a(\boldsymbol{k}) a^\dagger(\boldsymbol{k}) :\right) \\ &= \int d^3\boldsymbol{k}\, \frac{1}{2}\omega_{\boldsymbol{k}} \left(a^\dagger(\boldsymbol{k})\, a(\boldsymbol{k}) + a^\dagger(\boldsymbol{k})\, a(\boldsymbol{k})\right) \\ &= \int d^3\boldsymbol{k}\, \omega_{\boldsymbol{k}}\, a^\dagger(\boldsymbol{k})\, a(\boldsymbol{k}). \end{aligned}$$

Now with the normal ordered Hamiltonian, we will find that the infinite constant, E_0 disappears and the vacuum has zero energy.

$$\begin{aligned} :H: \,|0\rangle &= \int d^3\boldsymbol{k}\, \omega_{\boldsymbol{k}} a^\dagger(\boldsymbol{k})\, \underbrace{a(\boldsymbol{k})|0\rangle}_{=0} \\ &= 0. \end{aligned}$$

Using the normal ordering prescription, the energy eigenvalues (33) of the states become finite,

$$E' = \sum_{i=1}^{l} n_l\, \omega_{\boldsymbol{k}_i}.$$

Normal ordering will come very handy when we discus interacting scalar quantum field theory by means of perturbation theory and lead to a very important result, namely Wick's theorem.

Homework: Find out the normal ordered form of the operator $\mathcal{O} \equiv a(\boldsymbol{k}_1)\, a^\dagger(\boldsymbol{k}_2)\, a(\boldsymbol{k}_3)\, a^\dagger(\boldsymbol{k}_4)$ and work out the difference between $\mathcal{O}$ and $:\mathcal{O}:$