

PHYS 526 Notes #2: Quantizing the Scalar

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Having studied the classical theory of a real scalar field, we now apply quantum mechanics to it. Specifically, we will study the theory of the scalar $\phi(x)$ described at the classical level by the Lagrangian density

$$\mathcal{L} = \frac{1}{2}(\partial\phi)^2 - \frac{1}{2}m^2\phi^2 - \Lambda, \quad (1)$$

where Λ is a constant, independent of x and ϕ . Adding this constant does not affect the equations of motion. With this Lagrangian, we find the conjugate momentum

$$\Pi(x) = \partial_t\phi(x), \quad (2)$$

and the Hamiltonian

$$H = \int d^3x \left[\frac{1}{2}\Pi^2 + \frac{1}{2}(\vec{\nabla}\phi)^2 + \frac{1}{2}m^2\phi^2 + \Lambda \right]. \quad (3)$$

From this, we see that Λ represents a constant background energy density.

1 Mode Expansions

Before getting to quantization, it will be useful to look a bit more closely at the expansion of the classical field $\phi(x)$ described by the Lagrangian of Eq. (1) in terms of plane waves. Recall that the general solution to the classical equation of motion was

$$\phi(x) = \int \widetilde{d\mathbf{k}} \left[a(\vec{k})e^{-ik\cdot x} + a^*(\vec{k})e^{ik\cdot x} \right], \quad (4)$$

where $k^0 = E_{\mathbf{k}} = \sqrt{\vec{k}^2 + m^2}$. For the conjugate momentum $\Pi(x)$, this implies

$$\Pi(x) = \partial_t\phi(x) = -i \int \widetilde{d\mathbf{k}} k^0 \left[a(\vec{k})e^{-ik\cdot x} - a^*(\vec{k})e^{ik\cdot x} \right]. \quad (5)$$

We can also express the Hamiltonian in this way.

In formulating the quantum theory, it will be useful to solve for a and a^* in terms of ϕ and Π . To do this, recall that

$$\int d^3x e^{i\vec{p}\cdot\vec{x}} = (2\pi)^3 \delta^{(3)}(\vec{p}). \quad (6)$$

Multiplying $\phi(x)$ by $e^{ip\cdot x}$, with $p^0 = E_p = \sqrt{\vec{p}^2 + m^2}$, and integrating over d^3x , we get

$$\int d^3x e^{ip\cdot x} \phi(x) = \int d^3x \int \widetilde{d\mathbf{k}} \left[a(\vec{k})e^{-i(k^0-p^0)t} e^{i(\vec{k}-\vec{p})\cdot\vec{x}} + a^*(\vec{k})e^{i(k^0+p^0)t} e^{-i(\vec{p}+\vec{k})\cdot\vec{x}} \right] \quad (7)$$

$$= (2\pi)^3 \int \widetilde{d\mathbf{k}} \left[e^{-i(k^0-p^0)t} a(\vec{k})\delta^{(3)}(\vec{k}-\vec{p}) + e^{i(k^0+p^0)t} a^*(\vec{k})\delta^{(3)}(\vec{k}+\vec{p}) \right] \quad (8)$$

$$= \frac{1}{2p^0} a(\vec{p}) + \frac{1}{2p^0} a^*(-\vec{p})e^{2ip^0t}. \quad (9)$$

In going from the first to the second line, we have performed the $\int d^3x$ integration to obtain the delta functions of \vec{k} and \vec{p} . Note that $\vec{k} = \pm\vec{p}$ implies $k^0 = p^0 = \sqrt{\vec{p}^2 + m^2}$. A similar calculation on Π gives

$$\int d^3x e^{ip \cdot x} \Pi(x) = (-i)\frac{1}{2} a(\vec{p}) + (i)\frac{1}{2} a^*(-\vec{p}) e^{2ip^0 t} . \quad (10)$$

Taking linear combinations of these two results, we find

$$a(\vec{p}) = i \int d^3x e^{ip \cdot x} (\Pi - ip^0 \phi) , \quad (11)$$

$$a^*(\vec{p}) = -i \int d^3x e^{-ip \cdot x} (\Pi + ip^0 \phi) . \quad (12)$$

It is important to note that even though $\phi(x)$ and $\Pi(x)$ both depend on t , this dependence cancels out completely in these linear combinations.

2 Going Quantum

We are now set to formulate the quantum theory obtained from the classical field system described by the Lagrangian of Eq. (1). In the classical Hamiltonian formulation of the theory, Eq. (3), we have the conjugate variables $\phi(x)$ and $\Pi(x)$. To define a quantum theory, we elevate $\phi(x)$ and $\Pi(x)$ to Hermitian operators on a Hilbert space. As operators, they should satisfy commutation relations analogous to the classical Poisson brackets:

$$[\phi(t, \vec{x}), \phi(t, \vec{y})] = 0 = [\Pi(t, \vec{x}), \Pi(t, \vec{y})] \quad (13)$$

$$[\phi(t, \vec{x}), \Pi(t, \vec{y})] = i \delta^{(3)}(\vec{x} - \vec{y}) \quad (14)$$

These relations are a natural generalization of the Poisson brackets we obtained in the classical theory. Note as well that these commutation relations apply specifically when ϕ and Π are **evaluated at the same time** t .¹ This might seem a bit funny at first, but remember that we should think of \vec{x} as a label for different generalized coordinates (*i.e.* $\phi(t, \vec{x}) = q_{\vec{x}}(t)$), and that our Poisson bracket relations are defined specifically for functions of q_i and p_j evaluated at the same time value. For this reason, the relations of Eqs. (13,14) are sometimes called *equal-time commutation relations*.

At this point, it is worth going back to the mode expansions we found in Section 1 for the classical fields. With our quantum field operators, we can *define* time-independent operators $a(\vec{k})$ and $a^\dagger(\vec{k})$ according to

$$a(\vec{k}) = i \int d^3x e^{ik \cdot x} (\Pi - ik^0 \phi) |_{t=t_0} , \quad (15)$$

$$a^\dagger(\vec{k}) = -i \int d^3x e^{-ik \cdot x} (\Pi + ik^0 \phi) |_{t=t_0} , \quad (16)$$

¹Seriously, take note of this.

where $k^0 = E_k$ and all operators on the right-hand side are to be evaluated at the arbitrary reference time t_0 . At this point, we can also invert these relations to write $\phi(t_0, \vec{x})$ and $\Pi(t_0, \vec{x})$ in terms of $a(\vec{k})$ and $a^\dagger(\vec{k})$, but only at the fixed time t_0 . We will return to the issue of time dependence later on.

With the definitions of Eqs. (15,16), the commutation relations of ϕ and Π at t_0 imply simple commutation relations for a and a^\dagger :

$$\left[a(\vec{k}), a(\vec{p}) \right] = 0 = \left[a^\dagger(\vec{k}), a^\dagger(\vec{p}) \right], \quad (17)$$

$$\left[a(\vec{k}), a^\dagger(\vec{p}) \right] = (2\pi)^3 2k^0 \delta^{(3)}(\vec{k} - \vec{p}). \quad (18)$$

These relations should look familiar. Up to an overall normalization, they are equivalent to the commutation relations of the raising and lowering operators for a set of independent harmonic oscillators, $[a_i, a_j^\dagger] = i \delta_{ij}$. Using this analogy, we can build up the Hilbert space and find the energy eigenvalues.

The Hamiltonian of the system has the same form as the classical version, Eq. (3), but is now an operator built from the operators ϕ and Π . Rewriting it in terms of a and a^\dagger using ϕ and Π at time t_0 , we find

$$H = \frac{1}{2} \int \widetilde{d\vec{k}} k^0 \left[a^\dagger(\vec{k}) a(\vec{k}) + a(\vec{k}) a^\dagger(\vec{k}) \right] + \Lambda V \quad (19)$$

$$= \int \widetilde{d\vec{k}} k^0 a^\dagger(\vec{k}) a(\vec{k}) + \frac{1}{2} \int d^3k k^0 \delta^{(3)}(0) + \Lambda V, \quad (20)$$

where V is the volume of spacetime. The last two terms in the second line are formally infinite constants that do not affect the dynamics. We will assume that they cancel exactly. The remaining expression is just a continuous generalization of $H = \sum_{i=1}^N \omega_i a_i^\dagger a_i$, the Hamiltonian for a set of N independent oscillators.

Let's now build up the states. To do so, we make two assumptions:

1. There exists a unique vacuum state $|0\rangle$ such that

$$a(\vec{k})|0\rangle = 0 \quad (21)$$

for all values of \vec{k} .

2. Any operator on the Hilbert space can be built up from $\phi(x)$ and $\Pi(x)$. Equivalently, any local operator on the Hilbert space defined at time t_0 can be constructed out of $a(\vec{k})$ and $a^\dagger(\vec{k})$.

To build the Hilbert space, we will apply powers of $a^\dagger(\vec{k})$ to the vacuum.

Consider first the state $a^\dagger(\vec{p})|0\rangle := |\vec{p}\rangle$. Applying the Hamiltonian, we find

$$H|\vec{p}\rangle = \int \widetilde{d\vec{k}} k^0 a^\dagger(\vec{k}) a(\vec{k}) a^\dagger(\vec{p})|0\rangle \quad (22)$$

$$= \int \widetilde{d\vec{k}} k^0 a^\dagger(\vec{k}) \left[a^\dagger(\vec{p}) a(\vec{k}) + (2\pi)^3 2p^0 \delta^{(3)}(\vec{k} - \vec{p}) \right] |0\rangle \quad (23)$$

$$= 0 + p^0 |\vec{p}\rangle. \quad (24)$$

Therefore $|\vec{p}\rangle$ is an energy eigenstate with eigenvalue $p^0 = \sqrt{\vec{p}^2 + m^2}$. One can also show that this state is an eigenstate with eigenvalue \vec{p} of the spatial momentum operator $P^i = \int d^3x T^{0i} = - \int d^3x \Pi \partial_i \phi$ constructed from the energy momentum tensor (and generalized to quantum operators).

The physical interpretation of the state $|\vec{p}\rangle$ is that it represents a *particle* with three-momentum \vec{p} and energy $p^0 = \sqrt{\vec{p}^2 + m^2}$. In particular, the Lagrangian parameter m corresponds to the mass of the particle. This might come as a bit of a surprise. After all, we started with a continuous system, and we have ended up with discrete particle states. On the other hand, we already know that classical electromagnetism is a field theory that gives rises to particle excitations, photons, when quantized. Also, quantum mechanics is weird.

The most general state of the system is a linear combination of states of the form

$$[a^\dagger(\vec{k}_1)]^{n_1} [a^\dagger(\vec{k}_2)]^{n_2} \dots [a^\dagger(\vec{k}_N)]^{n_N} |0\rangle := |\vec{k}_1, n_1; \vec{k}_2, n_2; \dots; \vec{k}_N, n_N\rangle \quad (25)$$

This state has energy $E = \sum_{i=1}^N n_i k_i^0$ and three-momentum $\vec{P} = \sum_{i=1}^N n_i \vec{k}_i$. It is interpreted as a multiparticle state consisting of n_1 particles of momentum \vec{k}_1 , n_2 particles of momentum \vec{k}_2 , \dots , and n_N particles of momentum \vec{k}_N . Thus, we see that the field theory is able to describe any number of relativistic particles at once.

We can deduce three important properties of the particles described by this theory from the structure of the states. The first is that the particles have no identifying properties other than their momenta. They must therefore have spin zero. The second observation is that any number of particles can have the same momentum and there is no label to tell them apart. It follows that these particles are bosons. And third, the total energy of any multi-particle state is just the sum of the energies of the individual constituents. This implies that the particles do not interact with each other at all. For this reason, the simple quadratic theory we are studying is said to be a theory of *free particles* (or a free field theory). We will see later on that interactions between particles will emerge when we add higher-order terms to the Lagrangian.

3 More on Time Dependence

The operators we started with, $\phi(x) = \phi(t, \vec{x})$ and $\Pi(x) = \Pi(t, \vec{x})$, depend on time. We have also found quantum states $|\vec{k}_1, n_1; \dots; \vec{k}_N, n_N\rangle$ that are time-independent. Thus, we have been implicitly working in the Heisenberg picture of quantum mechanics where operators depend on time and states do not. Even so, there is a gap to fill. The ladder operators $a(\vec{k})$ and $a^\dagger(\vec{k})$ were constructed from ϕ and Π evaluated at the specific time t_0 , and so too was our Hamiltonian. We need to extend these results to arbitrary time values.

By assumption, time evolution in quantum mechanics is governed by the Hamiltonian. In particular, for any Heisenberg-picture operator $\mathcal{O}(t)$ we have

$$[H, \mathcal{O}] = -i\partial_t \mathcal{O} . \quad (26)$$

By applying this relation to successive infinitesimal time translations, one can show that it is equivalent to

$$\mathcal{O}(t) = e^{iH(t-t_0)}\mathcal{O}(t_0)e^{-iH(t-t_0)} . \quad (27)$$

Applying this general property to the ϕ and Π operators and using their commutation relations, we find

$$\partial_t\phi(t, \vec{x}) = i[H, \phi(t, \vec{x})] = \Pi(t, \vec{x}) , \quad (28)$$

$$\partial_t\Pi(t, \vec{x}) = i[H, \Pi(t, \vec{x})] = (\vec{\nabla}\phi)^2 - m^2\phi . \quad (29)$$

These reproduce the classical equations of motion. However, they are now to be interpreted as relations between time-dependent operators.

We also have

$$\phi(t, \vec{x}) = e^{iH(t-t_0)}\phi(t_0, \vec{x})e^{-iH(t-t_0)}, \quad \Pi(t, \vec{x}) = e^{iH(t-t_0)}\Pi(t_0, \vec{x})e^{-iH(t-t_0)} . \quad (30)$$

Now, recall that to construct the time-independent operators $a(\vec{k})$ and $a^\dagger(\vec{k})$, we used ϕ and Π defined at the fixed reference time t_0 . We can invert Eqs. (15,16) to solve for $\phi(t_0, \vec{x})$ and $\Pi(t_0, \vec{x})$, and then use Eq. (30) to find the operators defined at any time at all. Taking $t_0 = 0$, the result is²

$$\phi(t, \vec{x}) = \int \widetilde{d\vec{k}} \left[a(\vec{k})e^{-ik^0t+i\vec{k}\cdot\vec{x}} + a^\dagger(\vec{k})e^{ik^0t-i\vec{k}\cdot\vec{x}} \right] , \quad (31)$$

and similarly for $\Pi(t, \vec{x})$. While this relation looks just like what we had for the classical fields in Section 1, it is now a non-trivial relationship between quantum operators.

Finally let us mention that when we defined our Hamiltonian earlier, we did so only at the specific time $t_0 = 0$. However, since $\partial_t H = [H, H] = 0$, the Hamiltonian is time-independent and our earlier definition is valid for all t . This can be verified by plugging the general expansion of Eq. (31) into the expression for H in terms of $\phi(t, \vec{x})$ and $\Pi(t, \vec{x})$.

4 More on Operators

Before moving on to study more complicated Lagrangians, it is worth spending a bit more time with the quantum field operators in the free theory. We interpreted $|\vec{p}\rangle = a^\dagger(\vec{p})|0\rangle$ as a quantum state representing a single free particle with mass m and three-momentum \vec{p} . More generally, we found that the Hilbert space \mathcal{H} can be divided according to

$$\mathcal{H} = |0\rangle \oplus \{|1\rangle\} \oplus \{|2\rangle\} \oplus \dots , \quad (32)$$

where $\{|1\rangle\}$ represents the subspace of one-particle states, $\{|2\rangle\}$ the subspace of two-particle states, and so on.

²For other values of t_0 , one finds the same result but with $t \rightarrow (t - t_0)$.

Applying $\phi(x)$ to the vacuum, we find

$$\phi(x)|0\rangle = \int \widetilde{dk} e^{ik \cdot x} |\vec{k}\rangle . \quad (33)$$

The quantum field therefore creates a linear combination of one-particle states out of the vacuum. Let us also define the operator

$$\mathbb{I}_{1p} = \int \widetilde{dk} |\vec{k}\rangle \langle \vec{k}| . \quad (34)$$

It is not hard to show that this operator is the identity when acting on the subspace of one-particle states: $\mathbb{I}_{1p}|\vec{p}\rangle = |\vec{p}\rangle$.

There are two especially useful operations that can be defined for products of multiple operators. The first of these is called *normal ordering*, and applies specifically to the $a(\vec{k})$ and $a^\dagger(\vec{p})$ operators. A normal-ordered operator $N\{\mathcal{O}\}$ is one in which all the a^\dagger raising operators within it are written to the left of all a lowering operators. For example,

$$N\{a(\vec{k}_1)a^\dagger(\vec{k}_2)\} = a^\dagger(\vec{k}_2)a(\vec{k}_1) , \quad (35)$$

$$N\{[a^\dagger(\vec{k}_1)]^{n_1}[a(\vec{k}_2)]^{n_2}[(a^\dagger(\vec{k}_3)]^{n_3}\} = [a^\dagger(\vec{k}_1)]^{n_1}[a^\dagger(\vec{k}_3)]^{n_3}[a(\vec{k}_2)]^{n_2} . \quad (36)$$

The nice feature of a normal-ordered operator is that it has zero expectation value when sandwiched between $\langle 0|$ and $|0\rangle$ unless it is the identity. Furthermore, using the raising and lowering commutation relations, any operator can be written uniquely as a sum of normal-ordered operators, each containing an equal or smaller number of a and a^\dagger factors. Note that sometimes normal ordering is denoted by $:\mathcal{O}:$.

The second useful operation that applies to products of ϕ and Π operators is *time ordering*. For a pair of fields, the time-ordered product is

$$T\{\phi(t_1, \vec{x}_1)\phi(t_2, \vec{x}_2)\} = \Theta(t_1 - t_2)\phi(t_1, \vec{x}_1)\phi(t_2, \vec{x}_2) + \Theta(t_2 - t_1)\phi(t_2, \vec{x}_2)\phi(t_1, \vec{x}_1) , \quad (37)$$

where $\Theta(t)$ is the usual step function ($\Theta(t) = 1$ for $t > 0$, $\Theta(t) = 0$ for $t < 0$). Put another way, a time-ordered product of a pair of fields means that the field with the larger time is written to the left. More generally, the time-ordered product of multiple fields is the one where they are written in order of decreasing time values, from left to right.

The vacuum expectation value of the time-ordered product of a pair of fields will be of particular importance to us. Assuming $t_1 > t_2$, we have

$$\langle 0|T\{\phi(x_1)\phi(x_2)\}|0\rangle = \int \widetilde{dk} \int \widetilde{dp} \langle 0|a(\vec{k})a^\dagger(\vec{p})|0\rangle e^{-ik \cdot x_1} e^{ip \cdot x_2} \quad (38)$$

$$= \int \frac{d^3k}{(2\pi)^3} \frac{1}{2k^0} e^{-ik \cdot (x_1 - x_2)} \quad (39)$$

$$= \int \frac{d^3k}{(2\pi)^3} \int_{-\infty}^{\infty} \frac{dx}{(2\pi)} \frac{i}{x^2 - \vec{k}^2 - m^2 + i\epsilon} e^{-ix(t_1 - t_2) + i\vec{k} \cdot (\vec{x}_1 - \vec{x}_2)} . \quad (40)$$

In the last line, we have rewritten the preceding line using the integral relation you derived in hw-00. Note that the $i\epsilon$ picks out the pole at $x = k^0 = \sqrt{\vec{k}^2 + m^2}$ for $t_1 > t_2$. For $t_1 < t_2$,

it turns out that we obtain the same final result, but now the $i\epsilon$ selects the pole at $x = -k^0$ in the x integration. This expression is so important we give it a special name: the *Feynman propagator* D_F . It can be rewritten in the form

$$D_F(x - y) = \int \frac{d^4 p}{(2\pi)^4} \frac{i}{p^2 - m^2 + i\epsilon} e^{-ip \cdot (x-y)} , \quad (41)$$

where now p^0 is a free variable unrelated to $\sqrt{\vec{p}^2 + m^2}$.

We will see that the Feynman propagator describes a particle (or antiparticle) propagating from one point to another, possibly before and after scattering with other stuff. It also has a couple of useful properties. The first is that D_F is really simple if we Fourier transform it:

$$\int d^4 x e^{ik \cdot x} D_F(x) = \frac{i}{k^2 - m^2 + i\epsilon} := \tilde{D}_F(k) , \quad (42)$$

with k^0 still independent of $\sqrt{\vec{k}^2 + m^2}$. The second special property of the Feynman propagator is that it almost satisfies the Klein-Gordon equation:

$$(\partial^2 + m^2)D_F(x - y) = -i\delta^{(4)}(x - y) . \quad (43)$$

Because of this, D_F is said to be a Green's function of the Klein-Gordon equation.

5 Wave Functionals

We have constructed our quantum field theory in terms of states and operators in the Heisenberg picture. It can also be formulated in a way that is analogous to the wavefunction formulation of single-particle quantum mechanics in the Schrödinger picture. This formulation isn't used very much, but it's fun to see. More detailed accounts can be found in Refs. [3, 4].

Recall that for a single particle quantum system (in one dimension), we can define a position operator \hat{x} and eigenstates such that³

$$\hat{x}|x'\rangle = x'|x'\rangle , \quad \langle x'|x''\rangle = \delta(x' - x'') , \quad \mathbb{I} = \int dx' |x'\rangle \langle x'| . \quad (44)$$

The wavefunction of a state $|\Psi\rangle$ is then given by

$$\Psi(x) = \langle x|\Psi\rangle . \quad (45)$$

This generalizes straightforwardly to multiple spatial dimensions.

The analogous set of states in a quantum theory are

$$\hat{\phi}(0, \vec{x}) |\phi'\rangle = \phi'(\vec{x}) |\phi'\rangle . \quad (46)$$

³ Note that I've put a hat on the operator to distinguish it from the eigenvalue. I'll do so in this section for clarity, but nowhere else.

Here, $\hat{\phi}(0, \vec{x})$ is the field operator at $t = 0$ while $\phi'(\vec{x})$ is just a function that specifies the configuration of the field system at each point in space. Since $\hat{\phi}(0, \vec{x})$ is a Hermitian operator, these states form a complete set for the system, and the different eigenvalues are mutually orthogonal. Completeness translates into

$$\mathbb{I} = \int [\mathcal{D}\phi'] |\phi'\rangle \langle \phi'| . \quad (47)$$

Here, $\int [\mathcal{D}\phi']$ denotes a functional integral, in which all possible field configurations $\phi'(\vec{x})$ of the system are summed over. The statement of orthogonality takes the form

$$\langle \phi' | \phi'' \rangle = \delta[\phi' - \phi''], \quad (48)$$

where $\delta[f]$ is the delta functional, equal to zero unless $f = 0$ and infinite (in a controlled way) otherwise.⁴ The normalization of the delta functional is such that

$$\int [\mathcal{D}\phi'] \delta[\phi' - \phi''] F[\phi'] = F[\phi''] \quad (49)$$

for any functional F .

Given a quantum state $|\Psi\rangle$ of the theory, the corresponding *wavefunctional* is

$$\Psi[\phi'] = \langle \phi' | \Psi \rangle . \quad (50)$$

Alternatively, $\Psi[\phi']$ is just the expansion coefficient when expanding this state in the $\{|\phi'\rangle\}$ basis. We can also expand operators in this basis, and represent them as operators on wavefunctionals. The results for $\hat{\phi}(\vec{x})$ and $\hat{\Pi}(\vec{x})$ are

$$\hat{\phi}(0, \vec{x}) \rightarrow \phi(\vec{x}), \quad \hat{\Pi}(0, \vec{x}) \rightarrow -i \frac{\delta}{\delta \phi(\vec{x})} . \quad (51)$$

The ϕ case should be obvious, while for Π , note that for any functional $\Psi[\Phi]$

$$\left[\phi(\vec{x}), -i \frac{\delta}{\delta \phi(\vec{y})} \right] \Psi[\phi'] = i \delta^{(3)}(\vec{x} - \vec{y}) \Psi[\phi'] . \quad (52)$$

This is precisely the commutator we want.

With this functional representation in hand, we can now expand the general Schrödinger equation in the $\{|\phi'\rangle\}$ basis to obtain a Schrödinger equation for wavefunctionals. We have

$$i \frac{d}{dt} \Psi[\phi] = \frac{1}{2} \int d^3x \left(\left[-i \frac{\delta}{\delta \phi(\vec{x})} \right]^2 + (\vec{\nabla} \phi)^2 + m^2 \phi^2 \right) \Psi[\phi] . \quad (53)$$

This is nothing more than a continuous generalization of the simple harmonic oscillator.

⁴ Recall that a functional is an object that takes in a function and outputs a single number. A familiar example is the classical action $S[\phi]$.

References

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