Quantizing a Klein Gordon Field

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I first learned Quantum Mechanics through Leonard Susskind's Theoretical Minimum books. It was fascinating, but I wasn't entirely satisfied with it. I already knew the basics of special relativity when I read the book, and the quantum mechanics that Susskind described was inherently non-relativistic. I had an intense curiosity about how to make quantum mechanics relativistic. This began both my work in the Path Integral (see my other write-up, "Deriving the Canonical Quantization Approach from the Path Integral") and Quantum Field Theory. Early on, I tried to find a formula for how the fields would evolve in terms of the action. Susskind had already said that free fields followed wave equations. Unfortunately, I found many many permutations of the action, state vectors, and the vacuum vector that all reduced to the equation he had given when applied to a free field. In the end, I just brute-forced the problem, trying each equation until one started giving reasonable results. It's worth noting that everything here is work I did, and wrote up, in my Junior year. I have since found more efficient methods for some of this. Still, I thought I'd include it as a kind of "time capsule" of what I was obsessed with in eleventh grade.

We begin by defining a collection of operators (note here $c = \hbar = 1$):

$$\phi_n(t), \pi_n(t) \quad | \quad \forall t \quad [\phi_n(t), \pi_m(t)] = i\delta_{nm}$$

We will also assume the Lagrangian ($\mathcal{L}$) and Hamiltonian ($\mathcal{H}$) have the following form (here $V(\{\phi\})$ is an arbitrary potential that depends on all the ϕs):

$$\mathcal{L} = \sum_n \frac{1}{2}\dot{\phi}_n^2 - V(\{\phi\}), \quad \mathcal{H} = \sum_n \frac{1}{2}\dot{\phi}_n^2 + V(\{\phi\})$$

For this particular choice of Lagrangian and Hamiltonian we are going to prove that the following familiar equation is equivalent to Heisenberg's equation for the time dependence of an operator.

$$\frac{d}{dt}\frac{\partial \mathcal{L}}{\partial \dot{\phi}_n} - \frac{\partial \mathcal{L}}{\partial \phi_n} = 0 \quad \leftrightarrow \quad \dot{L} = i[H, L]$$

Though this at first glance might not seem general enough to be useful this is the form of both the Klein Gordon and Proca Lagrangians. For the sake of this proof we are going to assume that time evolution unfolds according to some unitary operator which is a function of all the ϕ_ns and π_ns:

$$\phi_n(t) = e^{itU(\{\phi\},\{\pi\})}\phi_n(0)e^{-itU(\{\phi\},\{\pi\})}, \quad \pi_n(t) = e^{itU(\{\phi\},\{\pi\})}\pi_n(0)e^{-itU(\{\phi\},\{\pi\})}$$

We are trying to show that, given the equation similar to stationary action above:

$$U(\{\phi\},\{\pi\}) = H(\{\phi\},\{\pi\})$$

First we write out the least action equation more explicitly in terms of the Lagrangian. We will divide it into two different equations, one to define the derivative of the generalized coordinate and the other to define the derivative of the momenta:

$$\frac{d}{dt}\frac{\partial \mathcal{L}}{\partial \dot{\phi}_n} - \frac{\partial \mathcal{L}}{\partial \phi_n} = 0 \quad \rightarrow \quad \dot{\pi}_n = -\frac{\partial V}{\partial \phi_n}, \quad \dot{\phi}_n = \pi_n$$

First, we need to write the first derivative of ϕ and π in terms of U (here ψ refers to an arbitrary operator, ϕ or π as both have the same time dependence and ϵ is a infinitesimal change in time small enough that it's higher powers are negligible):

$$\psi(t) = e^{itU}\psi_n(0)e^{-itU}$$

$$\psi(t+\epsilon) = \psi(t) + \epsilon\dot{\psi}(t) = e^{i\epsilon U}(e^{itU}\psi_n(0)e^{-itU})e^{-i\epsilon U}$$

We see that the interior of the parenthesis is just the definition of $\psi(t)$.

$$\psi(t) + \epsilon\dot{\psi}(t) = e^{i\epsilon U}\psi(t)e^{-i\epsilon U}$$

Expanding out the exponentials to first order in ϵ we get

$$\psi(t) + \epsilon\dot{\psi}(t) = (1 + i\epsilon U)\psi(t)(1 - i\epsilon U)$$

$$\psi(t) + \epsilon\dot{\psi}(t) = \psi(t) + i\epsilon U\psi(t) - i\epsilon\psi(t)U$$

Identifying $\dot{\psi}$ with the component of the right hand side of the expression proportional to ϵ we see that

$$\dot{\psi}(t) = i[U, \psi(t)]$$

This in turn means

$$\dot{\pi}_n(t) = i[U, \pi_n(t)], \quad \dot{\phi}_n(t) = i[U, \phi_n(t)]$$

To show that the Euler Lagrange equations above are equivalent to the Heisenberg time dependent operator equations we need to show that U is equal to the Hamiltonian. To do this we write out the component of the Euler Lagrange equations defining the change in π in terms of U:

$$\dot{\pi}_n = -\frac{\partial V}{\partial \phi_n} \quad \rightarrow \quad [U, \pi_n] = i\frac{\partial V}{\partial \phi_n}$$

Next we use the following equation which follows from the definition of the canonical commutator:

$$[F(\{\phi, \pi\}), \pi_n] = i\frac{\partial F}{\partial \phi_n}$$

Plugging this in and noting that U is a function of all the ϕ's and π's we get:

$$\frac{\partial U}{\partial \phi_n} = \frac{\partial V}{\partial \phi_n}$$

From this it follows that U has the following form where $K(\{\pi\})$ is an arbitrary function which depends only on the π's:

$$U(\{\pi, \phi\}) = K(\{\pi\}) + V(\{\phi\})$$

This is exactly the form we expect to see if $U = \mathcal{H}$: the potential energy plus something that depends only on the π's.

In order to pin down the form of K we need to use the second part of the Euler Lagrange equations, the part that defines the change in ϕ:

$$\dot{\phi}_n = \pi_n \quad \rightarrow \quad -i[\phi_n, U] = \pi_n$$

We need to use another equation that follows directly from the canonical, commutators:

$$[\phi_n, F(\{\phi, \pi\})] = i\frac{\partial F}{\partial \pi_n}$$

Plugging this in we get:

$$\frac{\partial U}{\partial \pi_n} = \frac{\partial K}{\partial \pi_n} = \pi_n$$

Up to a redundant additive constant this means K has the form:

$$K(\{\pi\}) = \sum_n \frac{1}{2}\pi_n^2$$

Plugging this into U we get:

$$U = K + V = \sum_n \frac{1}{2}\pi_n^2 + V(\{\phi\}) = \mathcal{H}$$

Thus:

$$U = \mathcal{H}$$

Now that we have shown the Euler Lagrange equations are equivalent to Heisenberg's equations for the time evolution of an operator, we can apply them to a simple quantum field theory. In this case we will use a Klein Gordon field with mass m. As before we work in natural units: $c = \hbar = 1$. The action is defined as follows (here the integral is over all four dimensions of space-time):

$$S = \int \frac{1}{2}(\partial_\mu \phi \partial^\mu \phi - m^2\phi^2)d^4X$$

Before we can leverage the Euler Lagrange equations on this field we need to do two things. The first is to derive the more useful field theoretic version of the Euler Lagrange equations from the originals above and the second is to justify our choice for the fields canonical commutators.

The derivation of the field theory Euler Lagrange equations from the originals is rather straight forward. First assume that the Lagrangian is the spatial integral over a Lagrangian density (note that from here on, the Lagrangian will be written L while the Lagrangian density will be $\mathcal{L}$):

$$L(t) = \int \mathcal{L}(\{\phi(\vec{x})\}, t) d^3x$$

We then write out the Euler Lagrange Equations using L:

$$\frac{\partial}{\partial t}\frac{\delta L}{\delta \dot{\phi}} - \frac{\delta L}{\delta \phi} = 0$$

Assuming that $\mathcal{L}(\{\phi, \partial\phi\})$ depends only on first derivatives of ϕ we can make the following two substitutions:

$$\frac{\delta L}{\delta \dot{\phi}} = \frac{\partial \mathcal{L}}{\partial \dot{\phi}} \quad \frac{\delta L}{\delta \phi} = -\sum_n \frac{\partial}{\partial x_n}\frac{\partial \mathcal{L}}{\partial[\frac{\partial \phi}{\partial x_n}]} + \frac{\partial \mathcal{L}}{\partial \phi}$$

Plugging this in and using the Einstein summation convention to simplify our notation (note that here X represents the 4-vector $X = (t, \vec{x})$):

$$\frac{\partial}{\partial X^\mu}\frac{\partial \mathcal{L}}{\partial[\frac{\partial \phi}{\partial X^\mu}]} - \frac{\partial \mathcal{L}}{\partial \phi} = 0$$

We will also need to justify our canonical commutators. The standard canonical commutators for some discrete collection of generalized coordinates $\{\phi_n\}$ are (remember that L represents the Lagrangian not the Lagrangian density):

$$[\phi_n, \frac{\partial L}{\partial \dot{\phi}_m}] = i\delta_{nm}$$

To generalize this to a continuous field we will need to reinterpret the partial derivative of the Lagrangian. To do this, we make the following definition of the partial derivative of a field:

$$\frac{\partial}{\partial \phi(\vec{x})} f(\phi(\vec{y})) = \begin{cases} f'(\phi(\vec{x})) & \vec{x} = \vec{y} \\ 0 & \vec{x} \neq \vec{y} \end{cases}$$

Let's use this, and the definition of L in terms of $\mathcal{L}$ to expand the following expression. What we are looking for is a form for $[\phi(x), \pi(y)]$:

$$[\phi(\vec{x}), \frac{\partial L}{\partial \dot{\phi}(\vec{x})}] = i$$

$$\int [\phi(\vec{x}), \frac{\partial \mathcal{L}(\vec{y})}{\partial \dot{\phi}(\vec{x})}] d^3x d^3y = i$$

$\frac{\partial \mathcal{L}}{\partial \dot{\phi}(\vec{x})}$ is only non-zero when $x = y$ so we can substitute x for y in that part of the expression yielding:

$$\int [\phi(\vec{x}), \frac{\partial \mathcal{L}(\vec{y})}{\partial \dot{\phi}(\vec{y})}] d^3x d^3y = i$$

From here we use the standard definition for the conjugate momentum of a field:

$$\pi(\vec{x}) = \frac{\partial \mathcal{L}}{\partial \dot{\phi}}(\vec{x})$$

Plugging this in we get:

$$\int [\phi(\vec{x}), \pi(\vec{y})] d^3x d^3y = i$$

However above we just said that the term $\frac{\partial \mathcal{L}}{\partial \dot{\phi}}$ is only non-zero when $\vec{x} = \vec{y}$ so we have:

$$\vec{x} \neq \vec{y} \quad [\phi(\vec{x}), \pi(\vec{y})] = 0$$

The only function that satisfies these two conditions is:

$$[\phi(\vec{x}), \pi(\vec{y})] = i\delta(\vec{x} - \vec{y})$$

Now that we have that out of the way we can use our equations on the Klein Gordon field. We plug our definition of the action into the Euler Lagrange equations:

$$\mathcal{L} = \frac{1}{2}(\partial_\mu \phi \partial^\mu \phi - m^2\phi^2) \qquad \frac{\partial}{\partial X^\mu} \frac{\partial \mathcal{L}}{\partial \frac{\partial \phi}{\partial X^\mu}} - \frac{\partial \mathcal{L}}{\partial \phi} = 0$$

$$(\partial_\mu \partial^\mu + m^2)\phi(\vec{x}) = 0$$

As expected we get the Klein Gordon equation. To solve this equation we write the field in terms of it's Fourier Transform (note that I've dropped some factors of 2π, had I included them they would have been divided out later in the analysis):

$$\phi(\vec{x},t) = \int \hat{\phi}(\vec{p},t)e^{i\vec{p}\cdot\vec{x}}d^3p$$

We can then plug this into the Klein Gordon equation and solve:

$$0 = (\partial_\mu\partial^\mu + m^2)\phi(\vec{x}) = (\frac{\partial^2}{\partial t^2} - \nabla^2 + m^2)\phi(\vec{x})$$

$$= \int \ddot{\hat{\phi}}(\vec{p},t)e^{i\vec{p}\cdot\vec{x}} - \hat{\phi}(\vec{p},t)\nabla^2 e^{i\vec{p}\cdot\vec{x}} + m^2\hat{\phi}(\vec{p},t)e^{i\vec{p}\cdot\vec{x}}d^3p$$

$$= \int [\ddot{\hat{\phi}}(\vec{p},t) + |\vec{p}|^2\hat{\phi}(\vec{p},t) + m^2\hat{\phi}(\vec{p},t)]e^{i\vec{p}\cdot\vec{x}}d^3p$$

This equation must hold for all values of $\vec{x}$ so we can drop the integral and evaluate for each momentum state individually:

$$\ddot{\hat{\phi}}(\vec{p},t) + |\vec{p}|^2\hat{\phi}(\vec{p},t) + m^2\hat{\phi}(\vec{p},t) = 0$$

$$\ddot{\hat{\phi}}(\vec{p},t) = -(|\vec{p}|^2 + m^2)\hat{\phi}(\vec{p},t)$$

This is just the equation for a simple harmonic oscillator with frequency $\sqrt{|\vec{p}|^2 + m^2}$ which has solutions:

$$\hat{\phi}(\vec{p},t) = A(\vec{p})e^{it\sqrt{|\vec{p}|^2+m^2}} + B(\vec{p})e^{-it\sqrt{|\vec{p}|^2+m^2}}$$

We will simplify this expression by calling the frequency E. Thus:

$$\hat{\phi}(\vec{p},t) = A(\vec{p})e^{itE} + B(\vec{p})e^{-itE}$$

We can then plug this back into our original form for the field operator:

$$\phi(\vec{x},t) = \int A(\vec{p})e^{iEt+i\vec{p}\cdot\vec{x}} + B(\vec{p})e^{-iEt+i\vec{p}\cdot\vec{x}}d^3p$$

We can then do a little rearranging, namely reversing the order over which we integrate the term involving $B(\vec{p})$:

$$\phi(\vec{x},t) = \int A(\vec{p})e^{iEt+i\vec{p}\cdot\vec{x}} + B(\vec{p})e^{-iEt+i\vec{p}\cdot\vec{x}}d^3p$$

$$= \int A(\vec{p}) e^{iEt + i\vec{p}\cdot\vec{x}} d^3p + \int B(\vec{p}) e^{-iEt + i\vec{p}\cdot\vec{x}} d^3p$$

$$= \int A(\vec{p}) e^{iEt + i\vec{p}\cdot\vec{x}} d^3p + \int B(-\vec{p}) e^{-iEt - i\vec{p}\cdot\vec{x}} d^3p$$

$$= \int A(\vec{p}) e^{iEt + i\vec{p}\cdot\vec{x}} + B(-\vec{p}) e^{-iEt - i\vec{p}\cdot\vec{x}} d^3p$$

To simplify our notation we can recognize that the term in the exponent is just the product of two 4-vectors, X and a new vector P defined $P = (E, \vec{p})$:

$$\phi(X) = \int A(\vec{p}) e^{iP_\mu X^\mu} + B(-\vec{p}) e^{-iP_\mu X^\mu} d^3p$$

Next we explicitly enforce the fact that the field $\phi(X)$ is a hermitian operator:

$$\phi^\dagger(X) = \phi(X)$$

$$\int A(\vec{p}) e^{iP_\mu X^\mu} + B(-\vec{p}) e^{-iP_\mu X^\mu} d^3p = \int A^\dagger(\vec{p}) e^{iP_\mu X^\mu} + B^\dagger(-\vec{p}) e^{-iP_\mu X^\mu} d^3p$$

Thus we can see:

$$A^\dagger(\vec{p}) = B(-\vec{p})$$

We can then plug this into our expression for the field to write it entirely in terms of the set of operators $A(\vec{p})$. In this form it is explicitly hermitian as it is written in as the sum of an operator and it's hermitian conjugate. Note that we are still integrating over d^3p and not over d^4P as the 0th component of the momentum 4-vector still depends on the others:

$$\phi(X) = \int A(\vec{p}) e^{iP_\mu X^\mu} + A^\dagger(\vec{p}) e^{-iP_\mu X^\mu} d^3p$$

Now that we have a form for $\phi(X)$ in terms of our new operator $A(\vec{p})$ we need to find the commutators of A. We are doing this because we are trying to find the particle creation and annihilation operators which should be hidden somewhere in the field.

We will do this by enforcing the canonical commutators while making two simplifying assumptions, namely that the only non-zero commutators those with an A and an $A^\dagger$ of the same momentum. This is of course only a guess and it will eventually be justified by the form we find for the energy. If the energy didn't reproduce the time dependence we'd found for A then we'd know that our assumptions had been inconsistent. As we will soon see they are not.

First we write out the canonical commutators for the field in position space:

$$[\phi(\vec{x}), \dot{\phi}(\vec{y})] = i\delta^3(\vec{x} - \vec{y})$$

We then plug in our form for the field in terms of A and simplify using the assumptions mentioned above:

$$i\delta^3(\vec{x} - \vec{y}) = \int\int 2iE[A(\vec{p}), A^\dagger(\vec{q})]e^{i(\vec{p}\cdot\vec{x} - \vec{q}\cdot\vec{y})}d^3p d^3q$$

This expression must only depend on $\vec{x} - \vec{y}$ and no other combination so this means $[A(\vec{p}), A^\dagger(\vec{q})]$ must be 0 whenever $\vec{p} \neq \vec{q}$. We can thus make the following definition:

$$[A(\vec{p}), A^\dagger(\vec{q})] = F(\vec{p})\delta^3(\vec{p} - \vec{q})$$

To find a form for F we plug it back into the above expression. Note that I've canceled the i on both sides of the expression:

$$\delta^3(\vec{x} - \vec{y}) = \int 2EF(\vec{p})e^{i\vec{p}\cdot(\vec{x} - \vec{y})}d^3p$$

In order for this integral to evaluate to the dirac delta our commutator must be:

$$[A(\vec{p}), A^\dagger(\vec{q})] = \frac{1}{16\pi^3 E}$$

We are looking for raising and lowering operators which have commutator 1. To this end we do the following manipulation:

$$[(4\sqrt{\pi^3 E}A(\vec{p})), (4\sqrt{\pi^3 E}A(\vec{p}))^\dagger] = 1$$

We can call the new operator $\psi(\vec{p})$ and rewrite the field in terms of it:

$$\psi(\vec{p}) = 4\sqrt{\pi^3 E}A(\vec{p})$$

$$\phi(X) = \int \left[\psi(\vec{p})e^{i(P_\mu X^\mu)} + \psi^\dagger(\vec{p})e^{-i(P_\mu X^\mu)}\right] \frac{d^3p}{4\sqrt{\pi^3 E}}$$

Though the ψs have the right commutators for creation and annihilation operators we are not done. We need to show that the operator they raise and lower is the energy and that they raise/lower by the right amount to be adding/removing particles. To do this, we will write out the energy in terms of ψ by using our definition of ϕ. The calculation is very long and not particularly enlightening so I will only show the end result here:

$$\mathcal{H} = \int E\psi^{\dagger}(\vec{p})\psi(\vec{p})d^3p$$

We have one more thing to do before we're done. We need to justify our assumptions from earlier about the form for the commutators of A and thus those of ψ. To do this, we can calculate the first derivatives of the ψs using Heisenbergs formula for time evolution. If it agrees with what we already have, than our assumptions were consistent.

$$\dot{\psi}(\vec{p}) = i[\mathcal{H}, \psi(\vec{p})] = -iE\psi(\vec{p})$$

This is the exact same equation we derived earlier for the time dependence of A. Thus the assumptions we made earlier related to the commutators of the ψs were correct.

Finally we can analyze the form we've found for the energy. The term in the middle is the number operator whose eigenvalues are raised and lowered by the ψs. We can interpret this as the number of particles of momentum $\vec{p}$. This is then multiplied by the energy of each of the particles. This is exactly the energy we would expect for a collection of non-interacting relativistic particles!

This is one of my favorite problems I've solved. It blows my mind that it's possible to start with the Klein Gordon equation, an equation for fields, and end up with a Hamiltonian that describes particles