Klein–Gordon Equation for the Quantum Fields

Thus far in class have introduced the (free) quantum scalar field \( \hat{\varphi}(x, t) \), its canonically conjugate quantum field \( \hat{\pi}(x, t) \), their equal-time commutation relations

\[
\begin{align*}
[\hat{\varphi}(x, t), \hat{\varphi}(x', \text{same } t)] &= 0, \\
[\hat{\pi}(x, t), \hat{\pi}(x', \text{same } t)] &= 0, \\
[\hat{\varphi}(x, t), \hat{\pi}(x', \text{same } t)] &= i\delta^{(3)}(x - x'),
\end{align*}
\]  

(1)

and the Hamiltonian

\[
\hat{H} = \int d^3x \left( \frac{1}{2} \hat{\pi}^2(x) + \frac{1}{2} (\nabla \hat{\varphi}(x))^2 + \frac{1}{2} m^2 \hat{\varphi}^2(x) \right). 
\]  

(2)

In this note I will show how the quantum version of the Klein-Gordon equation emerges from the Heisenberg equations

\[
\begin{align*}
i\frac{\partial \hat{\varphi}(x, t)}{\partial t} &= [\hat{\varphi}(x, t), \hat{H}], \\
i\frac{\partial \hat{\pi}(x, t)}{\partial t} &= [\hat{\pi}(x, t), \hat{H}].
\end{align*}
\]  

(3)

* * *

Note that in the Heisenberg picture, the Hamiltonian density operator

\[
\hat{\mathcal{H}}(x, t) = \frac{1}{2} \hat{\pi}^2(x, t) + \frac{1}{2} (\nabla \hat{\varphi}(x, t))^2 + \frac{1}{2} m^2 \hat{\varphi}^2(x, t)
\]  

(4)

is time dependent, although this dependence cancels out from the net Hamiltonian operator

\[
\hat{H}(t) = \int d^3x \hat{\mathcal{H}}(x, t) \equiv \text{same } \hat{H} \forall t
\]  

(5)

since \( i(d/dt)\hat{H} = [\hat{H}, \hat{H}] \equiv 0 \). Consequently, in the commutators

\[
\begin{align*}
[\hat{\varphi}(x, t), \hat{H}] &= \int d^3x' \left[ \hat{\varphi}(x, t), \hat{\mathcal{H}}(x', t') \right], \\
[\hat{\pi}(x, t), \hat{H}] &= \int d^3x' \left[ \hat{\pi}(x, t), \hat{\mathcal{H}}(x', t') \right]
\end{align*}
\]  

(6)

we may evaluate the Hamiltonian density \( \hat{\mathcal{H}}(x', t') \) at any time \( t' \) we like, as long it’s the same \( t' \) for all \( x' \). However, since we know the commutation relations (1) between the quantum
fields only at equal times \( t' = t \), we are naturally going to use \( \hat{H}(x', t) \) for the same time \( t \) as the field \( \phi(x, t) \) or \( \hat{\pi}(x, t) \) in the commutator (6), thus

\[
\left[ \hat{\phi}(x, t), \hat{H} \right] = \int d^3x' \left[ \hat{\phi}(x, t), \hat{H}(x', \text{same } t) \right] \quad (7)
\]

and

\[
\left[ \hat{\pi}(x, t), \hat{H} \right] = \int d^3x' \left[ \hat{\pi}(x, t), \hat{H}(x', \text{same } t) \right]. \quad (8)
\]

Let’s evaluate the first of these commutators. On the RHS of eq. (7) we have

\[
\left[ \hat{\phi}(x, t), \hat{H}(x', t) \right] = \frac{1}{2} \left[ \hat{\phi}(x, t), \hat{\pi}^2(x', t) \right] + \frac{1}{2} \left[ \hat{\phi}(x, t), (\nabla \hat{\phi}(x', t))^2 \right] + \frac{m^2}{2} \left[ \hat{\phi}(x, t), \hat{\phi}^2(x', t) \right]. \quad (9)
\]

Note that all fields here are taken at the same time \( t \), so all the \( \hat{\phi}(x, t) \) and \( \hat{\phi}(x', t) \) commute with each other. Consequently, the last two terms on the RHS of eq. (9) vanish:

\[
\forall \mathbf{x}, \mathbf{x}', \quad \left[ \hat{\phi}(x, t), \hat{\phi}(x', t) \right] = 0 \quad \Rightarrow \quad \left[ \hat{\phi}(x, t), \hat{\phi}^2(x', t) \right] = 0
\]

\[
\left[ \hat{\phi}(x, t), \nabla \hat{\phi}(x', t) \right] = \frac{\partial}{\partial x'} \left[ \hat{\phi}(x, t), \hat{\phi}(x', t) \right] = 0 \quad \Rightarrow \quad \left[ \hat{\phi}(x, t), (\nabla \hat{\phi}(x', t))^2 \right] = 0. \quad (10)
\]

In the remaining first term on the RHS of (9) we have

\[
\left[ \hat{\phi}(x, t), \hat{\pi}(x', t) \right] = i\delta^{(3)}(\mathbf{x}' - \mathbf{x}), \quad (11)
\]

which is a singular function of \( \mathbf{x} \) and \( \mathbf{x}' \) but as far as the Hilbert space of the quantum field theory, it’s just a c-number that commutes with all the quantum fields.* Consequently,

\[
\left[ \hat{\phi}(x, t), \hat{\pi}^2(x', t) \right] = \left\{ \left[ \hat{\phi}(x, t), \hat{\pi}(x', t) \right], \hat{\pi}(x', t) \right\} = 2i\delta^{(3)}(\mathbf{x}' - \mathbf{x}) \times \hat{\pi}(x', t) \quad (12)
\]

* In the Hilbert space of the quantum field theory, the operators are fields at different points, or modes of quantum fields, or polynomials and power series in fields or their modes, etc., etc. But the space coordinates such as \( \mathbf{x} \) or \( \mathbf{x}' \) where the fields act are not operators in this space but mere labels of the fields. Consequently, number-valued functions of \( \mathbf{x} \) and \( \mathbf{x}' \), or even singular functions such as \( \delta^{(3)}(\mathbf{x} - \mathbf{x}') \) are not operators but mere c-numbers — they commute with all the fields.
and therefore
\[ [\hat{\phi}(x, t), \hat{H}(x', t)] = i\delta^{(3)}(x' - x) \times \hat{\pi}(x', t). \]  
(13)

Integrating this commutator over the \( x' \) gives us
\[ [\hat{\phi}(x, t), \hat{H}] = \int d^3 x' i\delta^{(3)}(x' - x) \times \hat{\pi}(x', t) = i\hat{\pi}(x, t) \]  
(14)

and hence — by the Heisenberg equation for the \( \hat{\phi} \) field —
\[ \frac{\partial}{\partial t} \hat{\phi}(x, t) = \hat{\pi}(x, t), \]  
(15)

in perfect agreement with the classical Hamilton equation \( \frac{\partial}{\partial t} \phi(x, t) = \pi(x, t) \).

Now let’s evaluate the Heisenberg equation for the \( \hat{\pi} \) field. On the RHS of eq. (8) we have
\[ [\hat{\pi}(x, t), \hat{H}(x', t)] = \frac{1}{2} [\hat{\pi}(x, t), \hat{\pi}^2(x', t)] + \frac{1}{2} [\hat{\pi}(x, t), (\nabla \hat{\phi}(x', t))^2] + \frac{m^2}{2} [\hat{\pi}(x, t), \hat{\phi}^2(x', t)], \]  
(16)

and this time it’s the first term on the RHS that vanishes. Indeed, at equal times
\[ [\hat{\pi}(x, t), \hat{\pi}(x', t)] = 0 \Rightarrow [\hat{\pi}(x, t), \hat{\pi}^2(x', t)] = 0. \]  
(17)

For the third term (on the RHS of (16)), we have
\[ [\hat{\pi}(x, t), \hat{\phi}(x', t)] = -i\delta^{(3)}(x' - x), \]  
(18)

which is a singular function of \( x \) and \( x' \) but a c-number in the Hilbert space of the quantum fields, hence
\[ [\hat{\pi}(x, t), \hat{\phi}^2(x', t)] = -2i\delta^{(3)}(x' - x) \cdot \hat{\phi}(x', t). \]  
(19)

Finally, for the second term in (16) we have
\[ [\hat{\pi}(x, t), \nabla \hat{\phi}(x', t)] = \frac{\partial}{\partial x'} [\hat{\pi}(x, t), \hat{\phi}(x', t)] = -i\frac{\partial}{\partial x'} \delta^{(3)}(x' - x) \]  
(20)
— again, a very singular function of \( x \) and \( x' \) but a c-number in the Hilbert space, — so

\[
\left[ \hat{\pi}(x, t), (\nabla \hat{\phi}(x', t))^2 \right] = -2i \frac{\partial}{\partial x'} \delta^{(3)}(x' - x) \cdot \nabla \hat{\phi}(x', t). 
\]  

(21)

Altogether we have

\[
\left[ \hat{\pi}(x, t), \hat{H}(x', t) \right] = 0 - \frac{\partial}{\partial x'} \delta^{(3)}(x' - x) \cdot \nabla \hat{\phi}(x', t) - im^2 \delta^{(3)}(x' - x) \cdot \hat{\phi}(x', t) 
\]  

and hence

\[
\left[ \hat{\pi}(x, t), \hat{H} \right] = \int d^3x' \left( -i \frac{\partial}{\partial x'} \delta^{(3)}(x' - x) \cdot \nabla \hat{\phi}(x', t) - im^2 \delta^{(3)}(x' - x) \cdot \hat{\phi}(x', t) \right) 
\]  

\[
\langle \langle \text{integrating the first term by parts} \rangle \rangle 
\]

\[
= \int d^3x' i \delta^{(3)}(x' - x) \left( \nabla^2 \hat{\phi}(x', t) - m^2 \hat{\phi}(x', t) \right) 
\]

\[
= i \nabla^2 \hat{\phi}(x, t) - im^2 \hat{\phi}(x, t) \quad \langle \langle \text{@x rather than @x'} \rangle \rangle. 
\]  

(23)

Plugging this commutator into the Heisenberg equation for the \( \hat{\pi} \) field, we arrive at

\[
\frac{\partial}{\partial t} \hat{\pi}(x, t) = (\nabla^2 - m^2) \hat{\phi}(x, t). 
\]  

(24)

Finally, combining the two first-order (in \( \partial/\partial t \)) equations (15) and (24) for the quantum fields \( \hat{\phi} \) and \( \hat{\pi} \) we obtain the quantum version of the Klein–Gordon equation,

\[
\frac{\partial^2}{\partial t^2} \hat{\phi}(x, t) = \frac{\partial}{\partial t} \hat{\pi}(x, t) = (\nabla^2 - m^2) \hat{\phi}(x, t), 
\]  

(25)

or equivalently

\[
\left( \frac{\partial^2}{\partial t^2} - \nabla^2 + m^2 \right) \hat{\phi}(x, t) = 0. 
\]  

(26)