

# Klein–Gordon Equation for the Quantum Fields

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

$$\begin{aligned} [\hat{\phi}(\mathbf{x}, t), \hat{\phi}(\mathbf{x}', \text{same } t)] &= 0, \\ [\hat{\pi}(\mathbf{x}, t), \hat{\pi}(\mathbf{x}', \text{same } t)] &= 0, \\ [\hat{\phi}(\mathbf{x}, t), \hat{\pi}(\mathbf{x}', \text{same } t)] &= i\delta^{(3)}(\mathbf{x} - \mathbf{x}'), \end{aligned} \tag{1}$$

and the Hamiltonian

$$\hat{H} = \int d^3\mathbf{x} \left( \frac{1}{2}\hat{\pi}^2(\mathbf{x}) + \frac{1}{2}(\nabla\hat{\phi}(\mathbf{x}))^2 + \frac{1}{2}m^2\hat{\phi}^2(\mathbf{x}) \right). \tag{2}$$

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

$$i\frac{\partial\hat{\phi}(\mathbf{x}, t)}{\partial t} = [\hat{\phi}(\mathbf{x}, t), \hat{H}], \quad i\frac{\partial\hat{\pi}(\mathbf{x}, t)}{\partial t} = [\hat{\pi}(\mathbf{x}, t), \hat{H}]. \tag{3}$$

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Note that in the Heisenberg picture, the Hamiltonian density operator

$$\hat{\mathcal{H}}(\mathbf{x}, t) = \frac{1}{2}\hat{\pi}^2(\mathbf{x}, t) + \frac{1}{2}(\nabla\hat{\phi}(\mathbf{x}, t))^2 + \frac{1}{2}m^2\hat{\phi}^2(\mathbf{x}, t) \tag{4}$$

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

$$\hat{H}(t) = \int d^3\mathbf{x} \hat{\mathcal{H}}(\mathbf{x}, t) \equiv \text{same } \hat{H} \forall t \tag{5}$$

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

$$[\hat{\phi}(\mathbf{x}, t), \hat{H}] = \int d^3\mathbf{x}' [\hat{\phi}(\mathbf{x}, t), \hat{\mathcal{H}}(\mathbf{x}', t)], \quad [\hat{\pi}(\mathbf{x}, t), \hat{H}] = \int d^3\mathbf{x}' [\hat{\pi}(\mathbf{x}, t), \hat{\mathcal{H}}(\mathbf{x}', t)] \tag{6}$$

we may evaluate the Hamiltonian density  $\hat{\mathcal{H}}(\mathbf{x}', t')$  at any time  $t'$  we like, as long it's the same  $t'$  for all  $\mathbf{x}'$ . However, since we know the commutation relations (1) between the quantum

fields only at equal times  $t' = t$ , we are naturally going to use  $\widehat{\mathcal{H}}(\mathbf{x}', t)$  for the same time  $t$  as the field  $\hat{\phi}(\mathbf{x}, t)$  or  $\hat{\pi}(\mathbf{x}, t)$  in the commutator (6), thus

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

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

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

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

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

$$\begin{aligned} \forall \mathbf{x}, \mathbf{x}', \quad \left[ \hat{\phi}(\mathbf{x}, t), \hat{\phi}(\mathbf{x}', t) \right] = 0 &\implies \left[ \hat{\phi}(\mathbf{x}, t), \hat{\phi}^2(\mathbf{x}', t) \right] = 0 \\ &\Downarrow \\ \left[ \hat{\phi}(\mathbf{x}, t), \nabla \hat{\phi}(\mathbf{x}', t) \right] = \frac{\partial}{\partial \mathbf{x}'} \left[ \hat{\phi}(\mathbf{x}, t), \hat{\phi}(\mathbf{x}', t) \right] = 0 &\implies \left[ \hat{\phi}(\mathbf{x}, t), (\nabla \hat{\phi}(\mathbf{x}', t))^2 \right] = 0. \end{aligned} \quad (10)$$

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

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

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,

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

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\* 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

$$\left[ \hat{\phi}(\mathbf{x}, t), \hat{\mathcal{H}}(\mathbf{x}', t) \right] = i\delta^{(3)}(\mathbf{x}' - \mathbf{x}) \times \hat{\pi}(\mathbf{x}', t). \quad (13)$$

Integrating this commutator over the  $\mathbf{x}'$  gives us

$$\left[ \hat{\phi}(\mathbf{x}, t), \hat{H} \right] = \int d^3\mathbf{x}' i\delta^{(3)}(\mathbf{x}' - \mathbf{x}) \times \hat{\pi}(\mathbf{x}', t) = i\hat{\pi}(\mathbf{x}, t) \quad (14)$$

and hence — by the Heisenberg equation for the  $\hat{\phi}$  field —

$$\frac{\partial}{\partial t} \hat{\phi}(\mathbf{x}, t) = \hat{\pi}(\mathbf{x}, t), \quad (15)$$

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

Now let's evaluate the Heisenberg equation for the  $\hat{\pi}$  field. On the RHS of eq. (8) we have

$$\left[ \hat{\pi}(\mathbf{x}, t), \hat{\mathcal{H}}(\mathbf{x}', t) \right] = \frac{1}{2} \left[ \hat{\pi}(\mathbf{x}, t), \hat{\pi}^2(\mathbf{x}', t) \right] + \frac{1}{2} \left[ \hat{\pi}(\mathbf{x}, t), (\nabla \hat{\phi}(\mathbf{x}', t))^2 \right] + \frac{m^2}{2} \left[ \hat{\pi}(\mathbf{x}, t), \hat{\phi}^2(\mathbf{x}', t) \right], \quad (16)$$

and this time it's the first term on the RHS that vanishes. Indeed, at equal times

$$\left[ \hat{\pi}(\mathbf{x}, t), \hat{\pi}(\mathbf{x}', t) \right] = 0 \implies \left[ \hat{\pi}(\mathbf{x}, t), \hat{\pi}^2(\mathbf{x}', t) \right] = 0. \quad (17)$$

For the third term (on the RHS of (16)), we have

$$\left[ \hat{\pi}(\mathbf{x}, t), \hat{\phi}(\mathbf{x}', t) \right] = -i\delta^{(3)}(\mathbf{x}' - \mathbf{x}), \quad (18)$$

which is a singular function of  $\mathbf{x}$  and  $\mathbf{x}'$  but a c-number in the Hilbert space of the quantum fields, hence

$$\left[ \hat{\pi}(\mathbf{x}, t), \hat{\phi}^2(\mathbf{x}', t) \right] = -2i\delta^{(3)}(\mathbf{x}' - \mathbf{x}) \cdot \hat{\phi}(\mathbf{x}', t). \quad (19)$$

Finally, for the second term in (16) we have

$$\left[ \hat{\pi}(\mathbf{x}, t), \nabla \hat{\phi}(\mathbf{x}', t) \right] = \frac{\partial}{\partial \mathbf{x}'} \left[ \hat{\pi}(\mathbf{x}, t), \hat{\phi}(\mathbf{x}', t) \right] = -i \frac{\partial}{\partial \mathbf{x}'} \delta^{(3)}(\mathbf{x}' - \mathbf{x}) \quad (20)$$

— again, a very singular function of  $\mathbf{x}$  and  $\mathbf{x}'$  but a c-number in the Hilbert space, — so

$$\left[ \hat{\pi}(\mathbf{x}, t), (\nabla \hat{\phi}(\mathbf{x}', t))^2 \right] = -2i \frac{\partial}{\partial \mathbf{x}'} \delta^{(3)}(\mathbf{x}' - \mathbf{x}) \cdot \nabla \hat{\phi}(\mathbf{x}', t). \quad (21)$$

Altogether we have

$$\left[ \hat{\pi}(\mathbf{x}, t), \hat{\mathcal{H}}(\mathbf{x}', t) \right] = 0 - i \frac{\partial}{\partial \mathbf{x}'} \delta^{(3)}(\mathbf{x}' - \mathbf{x}) \cdot \nabla \hat{\phi}(\mathbf{x}', t) - im^2 \delta^{(3)}(\mathbf{x}' - \mathbf{x}) \cdot \hat{\phi}(\mathbf{x}', t) \quad (22)$$

and hence

$$\begin{aligned} \left[ \hat{\pi}(\mathbf{x}, t), \hat{H} \right] &= \int d^3 \mathbf{x}' \left( -i \frac{\partial}{\partial \mathbf{x}'} \delta^{(3)}(\mathbf{x}' - \mathbf{x}) \cdot \nabla \hat{\phi}(\mathbf{x}', t) - im^2 \delta^{(3)}(\mathbf{x}' - \mathbf{x}) \hat{\phi}(\mathbf{x}', t) \right) \\ &\quad \langle\langle \text{integrating the first term by parts} \rangle\rangle \\ &= \int d^3 \mathbf{x}' i \delta^{(3)}(\mathbf{x}' - \mathbf{x}) \left( \nabla^2 \hat{\phi}(\mathbf{x}', t) - m^2 \hat{\phi}(\mathbf{x}', t) \right) \\ &= i \nabla^2 \hat{\phi}(\mathbf{x}, t) - im^2 \hat{\phi}(\mathbf{x}, t) \quad \langle\langle @\mathbf{x} \text{ rather than } @\mathbf{x}' \rangle\rangle. \end{aligned} \quad (23)$$

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

$$\frac{\partial}{\partial t} \hat{\pi}(\mathbf{x}, t) = (\nabla^2 - m^2) \hat{\phi}(\mathbf{x}, t). \quad (24)$$

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,

$$\frac{\partial^2}{\partial t^2} \hat{\phi}(\mathbf{x}, t) = \frac{\partial}{\partial t} \hat{\pi}(\mathbf{x}, t) = (\nabla^2 - m^2) \hat{\phi}(\mathbf{x}, t), \quad (25)$$

or equivalently

$$\left( \frac{\partial^2}{\partial t^2} - \nabla^2 + m^2 \right) \hat{\phi}(\mathbf{x}, t) = 0. \quad (26)$$