Klein–Gordon Equation for the Quantum Fields

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

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

and the Hamiltonian

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

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

$$\widehat{\mathcal{H}}(\mathbf{x},t) = \tfrac{1}{2}\hat{\pi}^2(\mathbf{x},t) + \tfrac{1}{2}\big(\nabla\hat{\varphi}(\mathbf{x},t)\big)^2 + \tfrac{1}{2}m^2\,\hat{\varphi}^2(\mathbf{x},t) \tag{4}$$

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

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

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

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

we may evaluate the Hamiltonian density $\widehat{\mathcal{H}}(\mathbf{x}',t')$ 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 as the field $\hat{\pi}(\mathbf{x}, t)$ in the commutator (6), thus

$$\begin{aligned} \left[\hat{\phi}(\mathbf{x},t), \hat{H}\right] &= \int d^3\mathbf{x}' \left[\hat{\phi}(\mathbf{x},t), \widehat{\mathcal{H}}(\mathbf{x}', \text{same } t)\right] && (7) \\ \text{and} \quad \left[\hat{\pi}(\mathbf{x},t), \hat{H}\right] &= \int d^3\mathbf{x}' \left[\hat{\pi}(\mathbf{x},t), \widehat{\mathcal{H}}(\mathbf{x}', \text{same } t)\right]. && (8) \end{aligned}$$

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

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

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:

$$\begin{array}{ccc} \forall\mathbf{x},\mathbf{x}',\ \left[\hat{\phi}(\mathbf{x},t), \hat{\phi}(\mathbf{x}',t)\right] = 0 & \Longrightarrow & \left[\hat{\phi}(\mathbf{x},t), \hat{\phi}^2(\mathbf{x}',t)\right] = 0 \\ \Downarrow & & \\ \left[\hat{\phi}(\mathbf{x},t), \nabla\hat{\phi}(\mathbf{x}',t)\right] = 0 & \Longrightarrow & \left[\hat{\phi}(\mathbf{x},t), \left(\nabla\hat{\phi}(\mathbf{x}',t)\right)^2\right] = 0. \end{array} \tag{10}$$

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

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

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,

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

hence

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

⋆ 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

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

Finally, plugging this commutator into the Heisenberg equation for the $\hat{\phi}$ field we obtain

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

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

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

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

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

For the third term we have

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

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

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

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

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

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

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

Altogether we have

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

and hence

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

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

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

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,

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

or equivalently

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