Introduction to Quantum Fields

Hamiltonian Formalism

A classical field $\phi(\mathbf{x},t)$ is a continuous family of dynamical variables $\phi_{\mathbf{x}}(t)$. In the Hamiltonian formalism, each of these variables has its canonical momentum $\pi_{\mathbf{x}}(t)$, and the continuous family of these momenta form the *canonically conjugate field* $\pi(\mathbf{x},t)$. For multiple fields $\phi_i(\mathbf{x},t)$, each field has its own conjugate field $\pi_i(\mathbf{x},t)$. Most generally, the canonical fields obtain as *variational derivatives of the Lagrangian*

$$\pi_i(\mathbf{x}) \;=\; \frac{\delta L[\text{all}\,\phi_i\,\text{and all}\,\dot{\phi}_i\,@\text{all}\,\mathbf{x}]}{\delta\dot{\phi}_i(\mathbf{x})} \qquad\Longleftrightarrow\qquad \delta L[\text{due to}\ \delta\dot{\phi}_i] \;=\; \int\! d^3\mathbf{x}\,\pi_i(\mathbf{x})\delta\dot{\phi}_i(\mathbf{x}). \tag{1}$$

For a local Lagrangian

$$L \;=\; \int\! d^3\mathbf{x}\,\mathcal{L}(\phi_i, \nabla\phi_i, \dot{\phi}_i,\ \text{maybe}\ \nabla\dot{\phi}_i, \nabla\nabla\phi_i, \ldots, \ldots\ \forall i=1,\ldots,N), \tag{2}$$

the variational derivative (1) reduces to the ordinary derivatives of the Lagrangian density,

$$\pi_i(\mathbf{x}) \;=\; \frac{\delta L}{\delta\dot{\phi}_i(\mathbf{x})} \;=\; \frac{\partial\mathcal{L}}{\partial(\dot{\phi}_i)} \;-\; \nabla\cdot\frac{\partial\mathcal{L}}{\partial(\nabla\dot{\phi}_i)} \;+\; \cdots. \tag{3}$$

In relativistic field theories where the Lagrangian density depends only on the fields and their first spacetime derivatives, we have only the first term in this formula,

$$\pi_i(\mathbf{x},t) \;=\; \frac{\partial\mathcal{L}}{\partial(\dot{\phi}_i)}\,@(\mathbf{x},t). \tag{4}$$

In particular, for a relativistic scalar field with Lagrangian density

$$\mathcal{L}(\phi,\dot{\phi},\nabla\phi) \;=\; \tfrac{1}{2}(\dot{\phi})^2 \;-\; \tfrac{1}{2}(\nabla\phi)^2 \;-\; V(\phi) \tag{5}$$

(in $\hbar = c = 1$ units) the canonically conjugate field is simply

$$\pi \;=\; \frac{\partial\mathcal{L}}{\partial\dot{\phi}} \;=\; \dot{\phi}, \tag{6}$$

meaning $\pi(\mathbf{x},t) = \dot{\phi}(\mathbf{x},t)$.

The net energy H of a field configuration generalizes the mechanical formula $H = \sum_i p_i \dot{q}_i - L$ to

$$H = \int d^3\mathbf{x} \sum_i^{\text{fields}} \pi_i(\mathbf{x})\dot{\phi}_i(\mathbf{x}) - L, \tag{7}$$

Or in terms of the energy density

$$H = \int d^3\mathbf{x}\, \mathcal{H}(\mathbf{x}) \quad \text{where} \quad \mathcal{H} = \sum_i \pi_i \dot{\phi}_i - \mathcal{L}. \tag{8}$$

For example, for the relativistic scalar field with Lagrangian density (5), the energy density is

$$\mathcal{H} = \pi\dot{\phi} - \mathcal{L} = \tfrac{1}{2}(\dot{\phi})^2 + \tfrac{1}{2}(\nabla\phi)^2 + V(\phi). \tag{9}$$

Rephrasing this energy density in terms of the conjugate field π instead of the time derivative of ϕ, we obtain the Hamiltonian density

$$\mathcal{H}(\phi, \nabla\phi, \pi) = \tfrac{1}{2}\pi^2 + \tfrac{1}{2}(\nabla\phi)^2 + V(\phi) \tag{10}$$

and hence the net Hamiltonian

$$H[\phi(\mathbf{x}), \pi(\mathbf{x})] = \int d^3\mathbf{x}\, \mathcal{H}(\phi, \nabla\phi, \pi). \tag{11}$$

Consequently, the Hamilton equations for the relativistic scalar field and its canonical conjugate are

$$\frac{\partial\phi(\mathbf{x},t)}{\partial t} = + \left.\frac{\delta H}{\delta\pi(\mathbf{x})}\right|_t = \left.\frac{\partial\mathcal{H}}{\partial\pi}\right|_{(\mathbf{x},t)} = \pi(\mathbf{x},t) \tag{12}$$

while

$$\frac{\partial\pi(\mathbf{x},t)}{\partial t} = - \left.\frac{\delta H}{\delta\phi(\mathbf{x})}\right|_t = - \left.\left(\frac{\partial\mathcal{H}}{\partial\phi} - \nabla\cdot\frac{\partial\mathcal{H}}{\partial(\nabla\phi)}\right)\right|_{(\mathbf{x},t)} = \left(-\frac{dV}{d\phi} + \nabla\cdot\nabla\phi\right) @(\mathbf{x},t). \tag{13}$$

Together, these two equations are equivalent to the Euler–Lagrange equation

$$\frac{\partial^2\phi}{\partial t^2} = \frac{\partial\pi}{\partial t} = \nabla^2\phi - \frac{dV}{d\phi}. \tag{14}$$

Quantization

A classical field like $\phi(\mathbf{x},t)$ or $\pi(\mathbf{x},t)$ is a continuous family of dynamical variables $\phi_{\mathbf{x}}(t)$ or $\pi_{\mathbf{x}}(t)$ labeled by the space coordinates $\mathbf{x}=(x,y,z)$. In the quantum theory, each such dynamical variable becomes an operator in some Hilbert space, so we get *continuous families of operators* $\hat{\phi}_{\mathbf{x}}$ and $\hat{\pi}_{\mathbf{x}}$. In general, a quantum field is a continuous family of operators, one operator for each point $\mathbf{x}$ of space; in other words, *a quantum field is an operator-valued function of* $\mathbf{x}$ like $\hat{\phi}(\mathbf{x})$ or $\hat{\pi}(\mathbf{x})$.

Note that the Hilbert space of a QFT is not made of ordinary wavefunctions $\psi(\mathbf{x})$ but rather of the *wave functionals* $\psi[\phi(\mathbf{x})]$. Indeed, for a multi-particle system the wave function $\psi(\mathbf{x}_1,\ldots,\mathbf{x}_n)$ depends on all particles' positions rather than on a single $\mathbf{x}$, or for a system with $N=3n$ position variables $q_1,\ldots,q_N$ we have $\psi(q_1,\ldots,q_N)$. In a field theory, the discrete variables $q_1,\ldots,q_N$ become a continuous family $\phi_{\mathbf{x}}$, so the wave function becomes a functional of all the $\phi_{\mathbf{x}}$, thus $\psi[\phi(\mathbf{x})]$.

In practice, in quantum field theory people almost never bother with actual wave functional $\psi[\phi(\mathbf{x})]$ of quantum states, or with the wave functional action of various operators. Instead, we use the operator algebra to find the energy eigenstates of the free fields and to do the perturbations theory. This is analogous to how one can solve the harmonic oscillator — and do the perturbation theory in un-harmonic corrections — using nothing but the creation and the annihilation operators $\hat{a}^\dagger$ and $\hat{a}$ and the commutation relation $[\hat{a},\hat{a}^\dagger]=1$, which in turn follows from $[\hat{q},\hat{p}]=i\hbar$.

The time evolution of the quantum fields depends on the picture of quantum mechanics. In the Schrödinger picture, the operator-valued fields $\hat{\phi}(\mathbf{x})$ and $\hat{\pi}(\mathbf{x})$ do not depend on time so they are functions of $\mathbf{x}=(x,y,z)$ only. Instead, the time evolution comes through the time-dependent quantum states $|\psi\rangle\,(t)$. In the Heisenberg picture it's the other way around: the quantum states are time-independent while the operator-valued fields $\hat{\phi}(\mathbf{x},t)$ and $\hat{\pi}(\mathbf{x},t)$ evolve with time according to the Heisenberg equations

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

The commutators here obtain from the canonical commutation relations between the fields themselves. Generalizing the *equal-time* commutation relations between position and canonical momentum operators in ordinary QM

$$[\hat{q}_i(t), \hat{q}_j(\text{same}\, t)] \;=\; 0, \quad [\hat{p}_i(t), \hat{p}_j(\text{same}\, t)] \;=\; 0, \quad [\hat{q}_i(t), \hat{p}_j(\text{same}\, t)] \;=\; i\hbar\delta_{ij} \tag{16}$$

to continuous families of position-like operators $\hat{\phi}(\mathbf{x}, t)$ and momentum-like operators $\hat{\pi}(\mathbf{x}, t)$, we get

$$\begin{aligned} [\hat{\phi}(\mathbf{x}, t), \hat{\phi}(\mathbf{y}, \text{same}\, t)] &= 0, \\ [\hat{\pi}(\mathbf{x}, t), \hat{\pi}(\mathbf{y}, \text{same}\, t)] &= 0, \\ [\hat{\phi}(\mathbf{x}, t), \hat{\pi}(\mathbf{y}, \text{same}\, t)] &= i\delta^{(3)}(\mathbf{x} - \mathbf{y}) \end{aligned} \tag{17}$$

(in $c = \hbar = 1$ units). Note that these commutation relations work only at equal times. At un-equal times $t \neq t'$ we get much more complicated commutators

$$[\hat{\phi}(\mathbf{x}, t), \hat{\phi}(\mathbf{y}, t')] \;= ???, \quad [\hat{\pi}(\mathbf{x}, t), \hat{\pi}(\mathbf{y}, t')] \;= ???, \quad [\hat{\phi}(\mathbf{x}, t), \hat{\pi}(\mathbf{y}, t')] \;= ???, \tag{18}$$

that we generally do not know how to calculate. (Except for the free fields or order-by-order in perturbation theory).

Quantum Klein Gordon Equation

To illustrate the power of the equal-time commutation relations (17), let's use them to calculate the commutators in Heisenberg equations

$$i\frac{\partial}{\partial t}\hat{\phi}(\mathbf{x}, t) \;=\; [\hat{\phi}(\mathbf{x}, t), \hat{H}], \quad i\frac{\partial}{\partial t}\hat{\pi}(\mathbf{x}, t) \;=\; [\hat{\pi}(\mathbf{x}, t), \hat{H}] \tag{15}$$

for the free relativistic scalar field $\hat{\phi}(\mathbf{x}, t)$ and its conjugate $\hat{\pi}(\mathbf{x}, t)$, and then use those Heisenberg equations to derive the quantum version of the Klein–Gordon equation

$$\left(\frac{\partial^2}{\partial t^2} \;-\; \nabla^2 \;+\; m^2\right)\hat{\phi}(\mathbf{x}, t) \;=\; 0. \tag{19}$$

The classical free relativistic scalar field has Lagrangian density

$$\mathcal{L} \;=\; \frac{1}{2}\,\dot{\phi}^2 \;-\; \frac{1}{2}(\nabla\phi)^2 \;-\; \frac{m^2}{2}\,\phi^2 \tag{20}$$

and hence classical Hamiltonian density

$$\mathcal{H} \;=\; \frac{1}{2}\,\pi^2 \;+\; \frac{1}{2}(\nabla\phi)^2 \;+\; \frac{m^2}{2}\,\phi^2. \tag{21}$$

For the quantum theory, this gives the Hamiltonian density operator

$$\widehat{\mathcal{H}}(\mathbf{x},t) \;=\; \tfrac{1}{2}\hat{\pi}^2(\mathbf{x},t) \;+\; \tfrac{1}{2}\big(\nabla\hat{\phi}(\mathbf{x},t)\big)^2 \;+\; \tfrac{1}{2}m^2\,\hat{\phi}^2(\mathbf{x},t) \tag{22}$$

and hence the net Hamiltonian operator

$$\hat{H}(t) \;=\; \int\! d^3\mathbf{x}\,\widehat{\mathcal{H}}(\mathbf{x},t) \;\equiv\; \text{same } \hat{H}\ \forall t. \tag{23}$$

Note that the Hamiltonian density operator (22) is time dependent, although this time dependence cancels out from the net Hamiltonian operator $\hat{H}$ since $i(d/dt)\hat{H} = [\hat{H},\hat{H}] \equiv 0$. Consequently, in the commutators

$$\Big[\hat{\phi}(\mathbf{x},t),\hat{H}\Big] \;=\; \int\! d^3\mathbf{x}'\,\Big[\hat{\phi}(\mathbf{x},t),\widehat{\mathcal{H}}(\mathbf{x}',t')\Big], \qquad \Big[\hat{\pi}(\mathbf{x},t),\hat{H}\Big] \;=\; \int\! d^3\mathbf{x}'\,\Big[\hat{\pi}(\mathbf{x},t),\widehat{\mathcal{H}}(\mathbf{x}',t')\Big] \tag{24}$$

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 (17) 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 $\phi(\mathbf{x},t)$ or $\hat{\pi}(\mathbf{x},t)$ in the commutator (24), thus

$$\Big[\hat{\phi}(\mathbf{x},t),\hat{H}\Big] \;=\; \int\! d^3\mathbf{x}'\,\Big[\hat{\phi}(\mathbf{x},t),\widehat{\mathcal{H}}(\mathbf{x}',\text{same } t)\Big] \tag{25}$$

$$\text{and}\quad \Big[\hat{\pi}(\mathbf{x},t),\hat{H}\Big] \;=\; \int\! d^3\mathbf{x}'\,\Big[\hat{\pi}(\mathbf{x},t),\widehat{\mathcal{H}}(\mathbf{x}',\text{same } t)\Big]. \tag{26}$$

Let's evaluate the first of these commutators. On the RHS of eq. (25) we have

$$\Big[\hat{\phi}(\mathbf{x},t),\widehat{\mathcal{H}}(\mathbf{x}',t)\Big] \;=\; \frac{1}{2}\Big[\hat{\phi}(\mathbf{x},t),\hat{\pi}^2(\mathbf{x}',t)\Big] + \frac{1}{2}\Big[\hat{\phi}(\mathbf{x},t),\big(\nabla\hat{\phi}(\mathbf{x}',t)\big)^2\Big] + \frac{m^2}{2}\Big[\hat{\phi}(\mathbf{x},t),\hat{\phi}^2(\mathbf{x}',t)\Big]. \tag{27}$$

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. (27) vanish:

$$\begin{array}{ccc} \forall\mathbf{x},\mathbf{x}',\ \Big[\hat\phi(\mathbf{x},t),\hat\phi(\mathbf{x}',t)\Big] = 0 & \Longrightarrow & \Big[\hat\phi(\mathbf{x},t),\hat\phi^2(\mathbf{x}',t)\Big] = 0 \\ \Downarrow & & \\ \Big[\hat\phi(\mathbf{x},t),\nabla\hat\phi(\mathbf{x}',t)\Big] = \frac{\partial}{\partial\mathbf{x}'}\Big[\hat\phi(\mathbf{x},t),\hat\phi(\mathbf{x}',t)\Big] = 0 & \Longrightarrow & \Big[\hat\phi(\mathbf{x},t),\big(\nabla\hat\phi(\mathbf{x}',t)\big)^2\Big] = 0. \end{array} \tag{28}$$

In the remaining first term on the RHS of (27) we have

$$\Big[\hat\phi(\mathbf{x},t),\hat\pi(\mathbf{x}',t)\Big] = i\delta^{(3)}(\mathbf{x}'-\mathbf{x}), \tag{29}$$

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,

$$\Big[\hat\phi(\mathbf{x},t),\hat\pi^2(\mathbf{x}',t)\Big] = \Big\{\Big[\hat\phi(\mathbf{x},t),\hat\pi(\mathbf{x}',t)\Big],\hat\pi(\mathbf{x}',t)\Big\} = 2i\delta^{(3)}(\mathbf{x}'-\mathbf{x})\times\hat\pi(\mathbf{x}',t) \tag{30}$$

and therefore

$$\Big[\hat\phi(\mathbf{x},t),\widehat{\mathcal{H}}(\mathbf{x}',t)\Big] = i\delta^{(3)}(\mathbf{x}'-\mathbf{x})\times\hat\pi(\mathbf{x}',t). \tag{31}$$

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

$$\Big[\hat\phi(\mathbf{x},t),\hat H\Big] = \int\!d^3\mathbf{x}'\,i\delta^{(3)}(\mathbf{x}'-\mathbf{x})\times\hat\pi(\mathbf{x}',t) = i\hat\pi(\mathbf{x},t) \tag{32}$$

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

$$\frac{\partial}{\partial t}\hat\phi(\mathbf{x},t) = \hat\pi(\mathbf{x},t), \tag{33}$$

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

⋆ 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.

Now let's evaluate the Heisenberg equation for the $\hat{\pi}$ field. On the RHS of eq. (26) we have

$$\left[\hat{\pi}(\mathbf{x},t),\widehat{\mathcal{H}}(\mathbf{x}',t)\right] \;=\; \frac{1}{2}\left[\hat{\pi}(\mathbf{x},t),\hat{\pi}^2(\mathbf{x}',t)\right] + \frac{1}{2}\left[\hat{\pi}(\mathbf{x},t),\left(\nabla\hat{\phi}(\mathbf{x}',t)\right)^2\right] + \frac{m^2}{2}\left[\hat{\pi}(\mathbf{x},t),\hat{\phi}^2(\mathbf{x}',t)\right], \tag{34}$$

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

$$\left[\hat{\pi}(\mathbf{x},t),\hat{\pi}(\mathbf{x}',t)\right] \;=\; 0 \quad\Longrightarrow\quad \left[\hat{\pi}(\mathbf{x},t),\hat{\pi}^2(\mathbf{x}',t)\right] \;=\; 0. \tag{35}$$

For the third term (on the RHS of (34)), we have

$$\left[\hat{\pi}(\mathbf{x},t),\hat{\phi}(\mathbf{x}',t)\right] \;=\; -i\delta^{(3)}(\mathbf{x}'-\mathbf{x}), \tag{36}$$

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

$$\left[\hat{\pi}(\mathbf{x},t),\hat{\phi}^2(\mathbf{x}',t)\right] \;=\; -2i\delta^{(3)}(\mathbf{x}'-\mathbf{x})\cdot\hat{\phi}(\mathbf{x}',t). \tag{37}$$

Finally, for the second term in (34) we have

$$\left[\hat{\pi}(\mathbf{x},t),\nabla\hat{\phi}(\mathbf{x}',t)\right] \;=\; \frac{\partial}{\partial\mathbf{x}'}\left[\hat{\pi}(\mathbf{x},t),\hat{\phi}(\mathbf{x}',t)\right] \;=\; -i\frac{\partial}{\partial\mathbf{x}'}\delta^{(3)}(\mathbf{x}'-\mathbf{x}) \tag{38}$$

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

$$\left[\hat{\pi}(\mathbf{x},t),\left(\nabla\hat{\phi}(\mathbf{x}',t)\right)^2\right] \;=\; -2i\frac{\partial}{\partial\mathbf{x}'}\delta^{(3)}(\mathbf{x}'-\mathbf{x})\cdot\nabla\hat{\phi}(\mathbf{x}',t). \tag{39}$$

Altogether we have

$$\left[\hat{\pi}(\mathbf{x},t),\widehat{\mathcal{H}}(\mathbf{x}',t)\right] \;=\; 0 \;-\; i\frac{\partial}{\partial\mathbf{x}'}\delta^{(3)}(\mathbf{x}'-\mathbf{x})\cdot\nabla\hat{\phi}(\mathbf{x}',t) \;-\; im^2\delta^{(3)}(\mathbf{x}'-\mathbf{x})\cdot\hat{\phi}(\mathbf{x}',t) \tag{40}$$

and hence

$$\begin{aligned}\left[\hat{\pi}(\mathbf{x},t),\hat{H}\right] &= \int\!d^3\mathbf{x}'\left(-i\frac{\partial}{\partial\mathbf{x}'}\delta^{(3)}(\mathbf{x}'-\mathbf{x})\cdot\nabla\hat{\phi}(\mathbf{x}',t) \;-\; im^2\delta^{(3)}(\mathbf{x}'-\mathbf{x})\,\hat{\phi}(\mathbf{x}',t)\right)\\ &\qquad\langle\!\langle\,\text{integrating the first term by parts}\,\rangle\!\rangle\\ &= \int\!d^3\mathbf{x}'\,i\delta^{(3)}(\mathbf{x}'-\mathbf{x})\left(\nabla^2\hat{\phi}(\mathbf{x}',t) \;-\; m^2\hat{\phi}(\mathbf{x}',t)\right)\\ &= i\nabla^2\hat{\phi}(\mathbf{x},t) \;-\; im^2\hat{\phi}(\mathbf{x},t) \qquad \langle\!\langle\,@\mathbf{x}\text{ rather than }@\mathbf{x}'\,\rangle\!\rangle.\end{aligned} \tag{41}$$

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

$$\frac{\partial}{\partial t}\hat{\pi}(\mathbf{x},t) \;=\; \big(\nabla^2 - m^2\big)\hat{\phi}(\mathbf{x},t). \tag{42}$$

Finally, combining the two first-order (in $\partial/\partial t$) equations (33) and (42) for the quantum fields $\hat{\phi}$ and $\hat{\pi}$ we obtain the quantum version of the Klein–Gordon equation,

$$\frac{\partial^2}{\partial t^2}\hat{\phi}(\mathbf{x},t) \;=\; \frac{\partial}{\partial t}\hat{\pi}(\mathbf{x},t) \;=\; \big(\nabla^2 - m^2\big)\hat{\phi}(\mathbf{x},t), \tag{43}$$

or equivalently

$$\left(\frac{\partial^2}{\partial t^2} - \nabla^2 + m^2\right)\hat{\varphi}(\mathbf{x},t) \;=\; 0. \tag{44}$$