I. Canonical Operator Formalism of Quantum Mechanics

1.1 Canonical Quantization

Classical Mechanics:

Let $L(\dot{q},q)$ be a Lagrangian of a system, q being a dynamical variable and $\dot{q}$ its time derivative. The canonical momentum p is defined by

$$p = \frac{\partial L}{\partial \dot{q}} \tag{1.1}$$

and Hamiltonian of the system is given by the following Lagrange transform:

$$H(p,q) = p\,\dot{q} - L(\dot{q},q) \tag{1.2}$$

The Hamiltonian is a function of q and p only, because

$$\delta H = \delta(p\,\dot{q} - L) = (\delta p\,\dot{q} + p\delta\dot{q} - \frac{\partial L}{\partial q}\delta q - \frac{\partial L}{\partial \dot{q}}\delta\dot{q})$$

$$= (\delta p\,\dot{q} - \frac{\partial L}{\partial q}\delta q) \tag{1.3}$$

The Lagrange equation of motion

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}}\right) - \frac{\partial L}{\partial q} = 0 \tag{1.4}$$

is a consequence of Hamilton's principle:

$$\delta \int L\,dt = 0 \tag{1.5}$$

The Hamilton equations of motion are then derived from (1.1), (1.3) and (1.4) :

$$\dot{q} = \frac{\partial H}{\partial p}, \qquad \dot{p} = -\frac{\partial H}{\partial q} \tag{1.6}$$

The equation of motion for an arbitrary physical quantity F, is then obtained from (1.6) as

$$\dot{F} = \frac{\partial F}{\partial q}\dot{q} + \frac{\partial F}{\partial p}\dot{p} = \frac{\partial H}{\partial p}\frac{\partial F}{\partial q} - \frac{\partial F}{\partial p}\frac{\partial H}{\partial q} = [H, F]_P \tag{1.7}$$

where $[\ ,\ ]_P$ is the Poisson bracket defined by

$$[A, B]_P = -[B, A]_P = \frac{\partial A}{\partial p}\frac{\partial B}{\partial q} - \frac{\partial B}{\partial p}\frac{\partial A}{\partial q} \tag{1.8}$$

Quantum Mechanics :

In canonical operator formalism of quantum mechanics the dynamical variable $\hat{q}$ and its canonical conjugate momentum $\hat{p}$ are operators in a Hilbert space (from here on operators are denoted with $\hat{}$) and satisfy the following canonical commutation relation:

$$[\hat{q}, \hat{p}] \equiv \hat{q}\hat{p} - \hat{p}\hat{q} = i \tag{1.9}$$

The state of the system is a time dependent vector in the Hilbert space (Schrödinger picture), and the mechanical equation of the state vector is the Schrödinger equation:

$$i\frac{\partial}{\partial t} \,|\psi(t)\rangle = H(\hat{p}, \hat{q}) \,|\psi(t)\rangle \tag{1.10}$$

where H is a Hamiltonian operator obtained from the classical Hamiltonian (1.2) by promoting the classical variables to the quantum operator variables.

In this procedure there exists an ambiguity if p and q appear in a product form because of the noncommutativity of $\hat{p}$ and $\hat{q}$. If this is the case one must define the quantum mechanics by specifying the order of operators. Accordingly, to a classical system many quantum mechanical systems may correspond.

The operator ordering ambiguity may not be as serious a problem for systems of few degrees of freedoms. For systems of many degrees of freedom especially for field theories, however, this is a serious problem because the different ordering may produce different interaction vertices.

In this lecture, therefore, we assume that the Hamiltonian has the following standard form:

$$H = \frac{1}{2}\sum_{m=1}^{M} p_m^2 + V(q_1, q_2, \ldots\ldots, q_M) \tag{1.11}$$

which is of course free of operator ordering ambiguity and the quantization is unique.

1.2 Heisenberg Picture

In Schrödinger picture operators $\hat{q}$ and $\hat{p}$ are time independent while the state vector is time-dependent.

The Heisenberg picture is a picture in which the operators are time-dependent and the state vector is not. To be an equivalent quantum mechanical description the Heisenberg picture should be related to the Schrödinger picture by a time-dependent unitary transformation:

$$\hat{q}(t) = \hat{U}^{+}(t)\,\hat{q}\,\hat{U}(t), \qquad \hat{p}(t) = \hat{U}^{+}(t)\,\hat{p}\,\hat{U}(t) \tag{1.12}$$

$$|\,\Phi > = \hat{U}^{+}(t)\,|\,\psi(t)> \tag{1.13}$$

$$\hat{U}(t)\,\hat{U}^{+}(t) = \hat{U}^{+}(t)\,\hat{U}(t) = 1 \tag{1.14}$$

Using Schrödinger equation (1.10) we obtain the equation for $\hat{U}(t)$:

$$i\frac{\partial}{\partial t}\hat{U}(t) = \hat{H}\,\hat{U}(t) \tag{1.15}$$

A formal solution of $\hat{U}$ is

$$\hat{U}(t) = e^{-i\hat{H}t} \tag{1.16}$$

The coordinate representation is the representation in which $\hat{q}$ is diagonal:

$$\hat{q}\,|\,q> = |\,q>q \tag{1.17}$$

$$<q'\,|\,q> = \delta(q - q')$$

The Schrödinger wave function is a component of $|\,\psi(t)>$ in $|\,q>$ basis :

$$\psi(q, t) \equiv <q\,|\,\psi(t)> = <q\,|\,\hat{U}(t)\,|\,\Phi> \tag{1.18}$$

Similarly, in the Heisenberg picture we consider a moving basis $|\,q, t>$ such that the Schrödinger wave function $\psi(q, t)$ is a component of $|\,\Phi>$ in $|\,q, t>$ basis:

$$\psi(q,t) = \langle q,t \mid \Phi \rangle \tag{1.19}$$

Comparing with (1.18) we obtain

$$\mid q,t \rangle = \hat{U}^{+}(t) \mid q \rangle \tag{1.20}$$

The interpretation of $\psi(q,t)$ we adapt is the standard probability amplitude interpretation. The transition probability $q,t \to q',t'$ is then given by

$$\langle q',t' \mid q,t \rangle = \langle q' \mid \hat{U}(t')\,\hat{U}^{+}(t) \mid q \rangle = \langle q' \mid e^{-i(t'-t)\hat{H}} \mid q \rangle \tag{1.21}$$

Thus, we call $\hat{U}(t)$ the evolution operator.

1.3 Interaction Picture

We first split the Hamiltonian into two parts, free and interaction:

$$\hat{H} = \hat{H}_0 + \hat{H}_1 \tag{1.22}$$

We call $\hat{H}_0$ "free" part. But it need not be a free Hamiltonian provided it is a Hamiltonian for which we can solve the problem exactly. Next, construct the evolution operator due to H_0:

$$\hat{U}_0(t) = e^{-i\hat{H}_0 t} \tag{1.23}$$

The interaction representation is defined by

$$\hat{q}_I(t) = \hat{U}_0^{+}(t)\,\hat{q}\,\hat{U}_0(t), \qquad \hat{p}_I(t) = \hat{U}_0^{+}(t)\,\hat{p}\,\hat{U}_0(t) \tag{1.24}$$

$$\mid \psi_I(t) \rangle = \hat{U}_0^{+}(t) \mid \psi(t) \rangle \tag{1.25}$$

Using (1.23) and the Schrödinger equation we obtain

$$i\frac{\partial}{\partial t} \mid \psi_I(t) \rangle = \hat{H}_I(t) \mid \psi_I(t) \rangle \tag{1.26}$$

where

$$\hat{H}_I(t) = \hat{U}_0^{+}(t)\,\hat{H}_1\,\hat{U}_0(t) \tag{1.27}$$

A formal solution of (1.26) is given by

$$| \psi_I(t) > = T\, e^{-i\int_{-\infty}^{t} \hat{H}_I(t')dt'} \; | \psi_I(-\infty) >$$

$$\equiv \hat{U}_I\,(t, -\infty)\; | \psi_I\,(-\infty) > \tag{1.28}$$

where T is the time ordering symbol defined by

$$T(\hat{H}_I(t)\,\hat{H}_I(t')) = \hat{H}_I(t)\,\hat{H}_I(t') \quad \text{for } t > t'$$

$$= \hat{H}_I(t')\,\hat{H}_I(t) \quad \text{for } t < t' \tag{1.29}$$

etc.

Let $| n >$ be an eigenstate of H_0 with eigenvalue E_n :

$$\hat{H}_0\; | n > = E_n \; | n > \tag{1.30}$$

$| < n \mid \psi_I(t) > |^2$ is the probability of finding the system in n-state at t . Suppose at $t = -\infty$ the state is prepared in $| i >$ (initial) state:

$$| i > = \; | \psi_I(-\infty) > \tag{1.31}$$

The probability amplitude of finding the system in $| f >$ (final) at $t = \infty$ is given by

$$< f \; | \psi_I(\infty) > = \; < f \; | \; \hat{U}_I(\infty, -\infty) \; | i > \equiv \; < f \; | \hat{S} \; | i > \tag{1.32}$$

$\hat{S}$ is called the scattering operator (S-operator). Using (1.28) we obtain

$$\hat{S} = T\, e^{-i\int_{-\infty}^{\infty} \hat{H}_I(t)dt} \tag{1.33}$$

Using (1.21) and (1.25) we also obtain

$$\hat{S} = \lim_{\substack{t' \to \infty \\ t \to -\infty}} e^{i\hat{H}_0 t'} e^{-i\hat{H}(t'-t)} e^{-i\hat{H}_0 t} \tag{1.34}$$

1.4 Quantum Theory of Fields

The extension of the formalism described in the previous sections into many variables is trivially done by attaching an appropriate index to q and p .

$$q^m, \quad p^m \qquad (m = 1, 2, \ldots\ldots, M) \tag{1.35}$$

$$[\hat{q}^m, \hat{p}_n] = i\,\delta_{mn} \tag{1.36}$$

Field theories are systems of many (infinite) degrees of freedom. As an example let us consider a real scalar field theory whose Lagrangian density is given by

$$\mathcal{L} = \frac{1}{2}(\partial_\mu \phi \partial^\mu \phi - m^2 \phi) \tag{1.37}$$

where ϕ is a real scalar field which is a function of space-time point.

We restrict the space to a large finite volume V and $\phi(\vec{x},t)$ to satisfy the periodic boundary condition. We then expand ϕ into Fourier components:

$$\phi(\vec{x},t) = \frac{1}{V^{1/2}} \sum_{\vec{k}} e^{i\vec{k}\cdot\vec{x}} q_{\vec{k}}(t) \tag{1.38}$$

where momentum $\vec{k}$ is given by a set of integers n_x, n_y and n_z :

$$\vec{k} = \frac{2\pi}{L}\vec{n} \qquad (L^3 = V) \tag{1.39}$$

and $\sum_{\vec{k}}$ is the sum over n's. Note

$$q_{\vec{k}}^*(t) = q_{-\vec{k}}(t) \tag{1.40}$$

The Lagrangian of the system is then given by

$$L = \int_V d\vec{x}\,\mathcal{L} = \frac{1}{2}\sum_{\vec{k}}[\,|\dot{q}_{\vec{k}}(t)|^2 - \omega_k^2 |q_{\vec{k}}(t)|^2] \tag{1.41}$$

where

$$\omega_k^2 = \vec{k}^2 + m^2 \tag{1.42}$$

The Lagrangian (1.41) is equivalent to a system of free harmonic oscillators. Thus, the quantization is straightforward:

$$[\hat{q}_{\vec{k}}, \hat{p}_{\vec{k}'}] = i\,\delta_{\vec{k},-\vec{k}'} \tag{1.43}$$

where $p_{\vec{k}}$ is the canonical conjugate momentum :

$$p_{\vec{k}} = \dot{q}_{\vec{k}} \tag{1.44}$$

Using (1.38) and analogous expression for

$$\hat{\pi}(\vec{x}) = \frac{1}{V^{1/2}}\sum_{\vec{k}} e^{i\vec{k}\cdot\vec{x}}\hat{p}_{\vec{k}} \tag{1.45}$$

we obtain

$$[\hat{\phi}(\vec{x}),\, \hat{\pi}(\vec{x}\,')] = i\,\delta(\vec{x}-\vec{x}\,') \tag{1.46}$$

In deriving (1.46) we used

$$\frac{1}{V}\sum_{\vec{k}} = \frac{1}{(2\pi)^3}\int d\vec{k} \tag{1.47}$$

which is valid in the infinite volume limit.

The Hamiltonian of the system is given by

$$\hat{H} = \frac{1}{2}\sum_{\vec{k}}(\hat{p}_{\vec{k}}^{\,2} + \omega_k^2\hat{q}_{\vec{k}}^{\,2}) \tag{1.48}$$

$$= \frac{1}{2}\int d\vec{x}\,(\hat{\pi}^2(\vec{x}) + (\vec{\nabla}\hat{\phi}(\vec{x}))^2 + m^2\hat{\phi}^2(\vec{x})) \tag{1.49}$$

$$\equiv \frac{1}{2}\int d\vec{x}\,\hat{\pi}^2(\vec{x}) + V[\hat{\phi}] \tag{1.50}$$

Although we started with the Lorentz invariant Lagrangian density (1.37) the canonical operator formalism is inherently non-covariant, since the time is treated in the canonical formalism entirely differently from the space. The shortcoming of the non-covariance is remedied to some extent in the Heisenberg picture:

$$\hat{\phi}(\vec{x},t) = e^{i\hat{H}t}\,\hat{\phi}(\vec{x})e^{-i\hat{H}t}, \qquad \hat{\pi}(\vec{x},t) = e^{i\hat{H}t}\,\hat{\pi}(\vec{x})e^{-i\hat{H}t}$$

Using the explicit form of $\hat{H}$ we obtain

$$\partial_t\hat{\phi}(\vec{x},t) = \hat{\pi}(\vec{x},t), \qquad \partial_t\hat{\pi}(\vec{x},t) = (\nabla^2 + m^2)\hat{\phi}(\vec{x},t)$$

accordingly a covariant equation follows:

$$(\partial_t^2 - \nabla^2 + m^2)\hat{\phi}(\vec{x},t) \equiv (\Box + m^2)\hat{\phi}(x) = 0 \tag{1.51}$$

We demonstrated the Lorentz covariance of Heisenberg picture for a free scalar field. Convince yourself this is so with interactions provided that the interaction Lagrangian does not involve space-time derivatives.