Section 5.3: Classical Commutation Relations

The Hamiltonian is the primary quantity of interest for quantum theory. The specification of a quantum mechanical Hamiltonian follows several steps

(1) Determine the classical Hamiltonian
(2) Substitute operators for the classical dynamical variables (e.g., p's and q's)
(3) Specify the commutation relations between those operators

The commutation relations in quantum mechanics somewhat resemble the Poisson brackets in classical mechanics. The commuation relations and Poisson brackets determine the evolution of the dynamical variables. In the quantum theory, operators replace the classical dynamical variables. In fact, the Heisenberg quantum picture has the greatest resemblance to classical mechanics because the operators carry the system dynamics. In quantum theory, the commutation relations give time derivatives of operators. A commutator is defined by $\left[\hat{A},\hat{B}\right]=\hat{A}\hat{B}-\hat{B}\hat{A}$ where $\hat{A},\hat{B}$ are operators. The Poisson bracket as the classical version, uses partial derivatives whereas the quantum mechanical commutator does not.

Definition: Let $A=A(q_i,p_i)$ $B=B(q_i,p_i)$ be two differentiable functions of the generalized coordinates and momentum. We define the Poisson brackets by

$$[A,B]=\sum_i\left[\frac{\partial A}{\partial q_i}\frac{\partial B}{\partial p_i}-\frac{\partial B}{\partial q_i}\frac{\partial A}{\partial p_i}\right]$$

Sometimes we subscript the brackets with p,q

$$[A,B]=[A,B]_{q,p}$$

to indicate Poisson brackets. Using the definition of Poisson brackets, some basic properties can be proved.

(1) Let A, B be functions of the phase space coordinates q,p and let c be a number then

$$[A,A]=0 \qquad [A,B]=-[B,A] \qquad [A,c]=0$$

(2) Let A, B, C be differentiable functions of the phase space coordinates q,p then

$$[A+B,C]=[A,C]+[B,C] \qquad [AB,C]=A[B,C]+[A,C]B$$

(3) The time evolution of the dynamical variable A (for example) can be calculated by

$$\frac{dA}{dt}=[A,H]+\frac{\partial A}{\partial t}$$

Proof:

$$\frac{dA}{dt}=\sum_i\left[\frac{\partial A}{\partial q_i}\frac{dq_i}{dt}+\frac{\partial A}{\partial p_i}\frac{dp_i}{dt}\right]+\frac{\partial A}{\partial t}$$

We include the partial with respect to time in case the function A explicitly depends on time. Substituting the two relations for the rate of change of position and momentum

$$\frac{dq_i}{dt} = \frac{\partial H}{\partial p_i} \qquad \frac{dp_i}{dt} = -\frac{\partial H}{\partial q_i}$$

the Poisson brackets become

$$\frac{dA}{dt} = \sum_i \left[\frac{\partial A}{\partial q_i}\frac{\partial H}{\partial p_i} - \frac{\partial A}{\partial p_i}\frac{\partial H}{\partial q_i} \right] + \frac{\partial A}{\partial t} = [A, H] + \frac{\partial A}{\partial t}$$

Although the order of multiplication AH=HA does not matter in classical theory, the order must be maintained in quantum theory. In quantum theory, the order of two operators can only be switched by using the commutation relations.

(4) $\dot{q}_m = [q_m, H] \qquad \dot{p}_m = [p_m, H]$

Proof: Consider the first one for example

$$[q_m, H] = \sum_i \left[\frac{\partial q_m}{\partial q_i}\frac{\partial H}{\partial p_i} - \frac{\partial q_m}{\partial p_i}\frac{\partial H}{\partial q_i} \right] = \sum_i \left[\delta_{im}\frac{\partial H}{\partial p_i} - 0\frac{\partial H}{\partial q_i} \right] = \frac{\partial H}{\partial p_m} = \dot{q}_m$$

(5) $[q_i, q_j] = 0 \quad [p_i, p_j] = 0 \quad [q_i, p_j] = \delta_{ij}$