Quantum Mechanics I

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1 Classical Mechanics

In order to later compare quantum mechanics, let us first introduce some classical mechanics.

In classical mechanics, we study classical objects/particles which has a mass $m \in \mathbb{R}$ and a state. In particular, the state of the particle is represented by its position, commonly $r \in \mathbb{R}^3$, and its velocity $v = \dot{r} \in \mathbb{R}^3$. More conveniently, we can also represent the velocity in terms of its momentum $p = mv$.

We recall Newton's second law which describes how the state of a particle changes in time in the presence of external forces. That is,

$$\dot{p} = F(r),$$

where F is the external force depending on r.

As the state of a particle is represented by its position and momentum, visually the state of a particle can be represented by a phase-space with a trajectory corresponding to $(r(t), p(t))$.

An another formulation of classical mechanics is Hamilton's formulation. While Hamilton's formulation is very powerful, it does not apply to every classical system. In particular, Hamilton's formulation requires the system to be conservative.

Definition 1.1 (Conservative)**.** A classical system is said to be conservative if

$$F(r) = -\nabla V(r),$$

where V is the potential given the position.

Definition 1.2 (Hamiltonian Function)**.** The Hamiltonian function H is defined as

$$H(p, q) = \frac{p^2}{2m} + V(q),$$

where $p^2/2m$ is the kinetic energy and V the potential.

Thus, with the definition of conservative in mind, we see that for a one dimensional system with position given by $q \in \mathbb{R}$, we have

$$\dot{p} = F(q) = -\frac{\partial V}{\partial q} \text{ and } \dot{q} = \frac{p}{m}.$$

Writing in terms of the Hamiltonian function, we obtain,

$$\dot{p} = -\frac{\partial H}{\partial q} \text{ and } \dot{q} = \frac{\partial H}{\partial p}.$$

These two equations are known as Hamilton's canonical equations and describe the motion of a particle in a conservative system. The theory itself is more general in which we simply require p, q to be canonically conjugate variables.

Example 1.1 (Free Particle)**.** Consider a free particle with $V(q) = 0$ (thus, $H = p^2/2m$), we have the canonical equations $\dot{p} = 0$ and $\dot{q} = p/m$, and thus, $p(t) = p(0)$ and $q(t) = q(0) + \frac{p}{m}t$.

Example 1.2 (Harmonic Oscillator)**.** A harmonic oscillator is described by $V(q) \propto q^2$. By similar calculation we find $\ddot{q} = -\frac{2k}{m}q$ for some k such that $V = kq^2$.

1.1 Poisson Brackets

As for a particle in classical mechanics, the state is given by its position and momentum, any measurable quantity A is given as a function $A(p, q)$ such that

$$\frac{\mathrm{d}A}{\mathrm{d}t} = \frac{\partial A}{\partial p}\dot{p} + \frac{\partial A}{\partial q}\dot{q} + \frac{\partial A}{\partial t}.$$

Substituting the Hamiltonian equations, we have

$$\frac{\mathrm{d}A}{\mathrm{d}t} = -\frac{\partial A}{\partial p}\frac{\partial H}{\partial q} + \frac{\partial A}{\partial q}\frac{\partial H}{\partial p} + \frac{\partial A}{\partial t} = \frac{\partial A}{\partial q}\frac{\partial H}{\partial p} - \frac{\partial A}{\partial p}\frac{\partial H}{\partial q} + \frac{\partial A}{\partial t}.$$

As the first term of this equation is very common, we denote it as $\{H, A\}$ such that

$$\frac{\mathrm{d}A}{\mathrm{d}t} = \{H, A\} + \frac{\partial A}{\partial t}.$$

Similarly, for general variables F, G,

$$\{F, G\} := \sum_{n=1}^{N} \frac{\partial F}{\partial p_n}\frac{\partial G}{\partial q_n} - \frac{\partial F}{\partial q_n}\frac{\partial G}{\partial q_n},$$

and is known as the Poisson bracket of F and G.

Definition 1.3 (Poisson Bracket)**.** A Poisson bracket is simply any bracket of functions satisfying

- $\{A, A\} = 0$;
- $\{c_1 A + c_2 B, C\} = c_1\{A, C\} + c_2\{B, C\}$;
- $\{A, B\} = -\{B, A\}$.
- $\{c, A\} = 0$ for any constant c;
- $\{AB, C\} = A\{B, C\} + \{A, C\}B$ (Leibniz rule);
- $\{A, \{B, C\}\} + \{B, \{C, A\}\} + \{C, \{A, B\}\} = 0$ (Jacobi identity).

As an exercise, one may check that the Poisson bracket defined above is indeed a Poisson bracket.

Proposition 1.1. $\{p, q\} = 1$ and in higher dimensions. $\{p_i, q_j\} = \delta_{ij}$.

Definition 1.4 (Canonical Conjugate Variables)**.** $P(p, q), Q(p, q)$ are called canonical conjugate variables if $\{P, Q\} = 1$. Similarly, for higher dimensions, P, Q are canonical conjugates if $\{P_i, Q_j\} = \delta_{ij}$.

Proposition 1.2. For any pair of canonical conjugate variables P, Q, we have

$$\dot{P}_j = -\frac{\partial H}{\partial Q_j} = \{H, P_j\} \text{ and } \dot{Q}_j = \frac{\partial H}{\partial P_j} = \{H, Q_j\}.$$