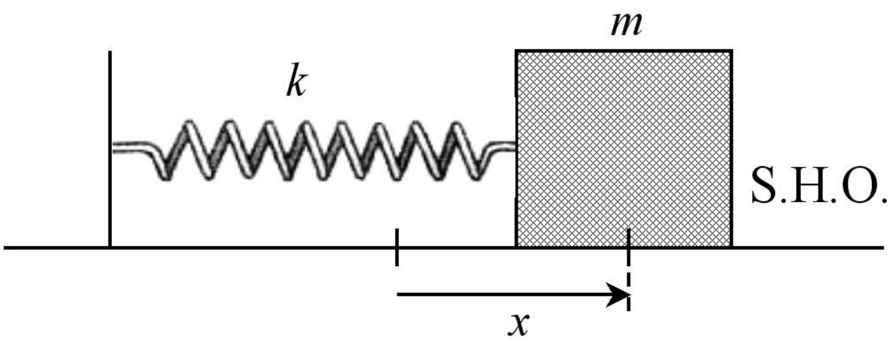
Chapter 2

Brief Review of Classical Mechanics and Quantum States



x: displacement from the equilibrium position

2.1 Newtonian Mechanics

Newton's Equation of Motion:

$$m\ddot{x} = F(x) = -kx \tag{2.1}$$

$$\uparrow \qquad \uparrow$$

$$\text{effect} \quad \text{cause}$$

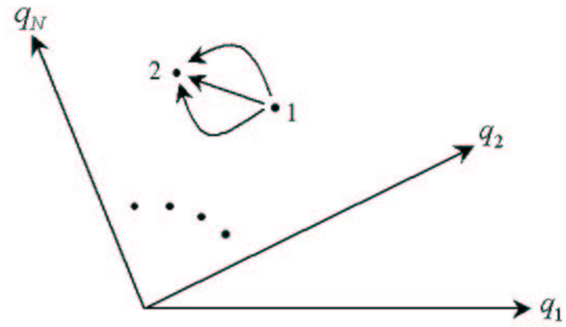
$$\therefore \quad \ddot{x} \ + \omega_0^2 x = 0; \quad \omega_0 = \sqrt{\frac{k}{m}} \tag{2.2}$$

2.2 Lagrangian Mechanics

$$\text{Lagrangian} \qquad L \equiv T(K.E.) - U(P.E.) \tag{2.3}$$

$$\therefore \qquad L = \frac{1}{2}m\dot{x}^2 - \frac{1}{2}kx^2 \tag{2.4}$$

Stationary Action Principle (Hamilton's principle):



Configurational Space

$$q = (q_1, \cdots, q_N)\text{: generalized coordinates}$$
$$\dot{q} = (\dot{q}_1, \cdots, \dot{q}_N)$$

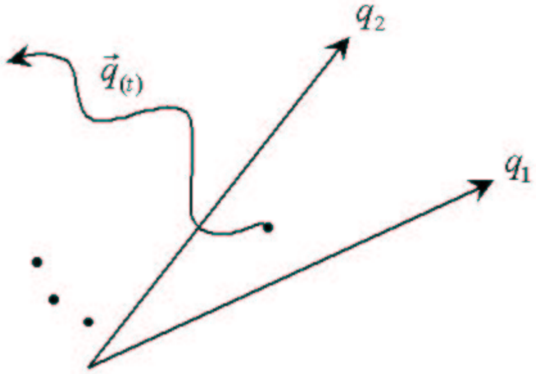
$$\begin{aligned}
\text{Action} \;\; A(\overrightarrow{q}) &\equiv \int_{t_1}^{t_2} L(q, \dot{q}, t) dt \\
\delta A &= \int_{t_1}^{t_2} \sum_i [\frac{\partial L}{\partial g_i} \delta q_i + \frac{\partial L}{\partial \dot{q}_i} \delta \dot{q}_i] dt \\
\delta \dot{q}_i &= \delta(\frac{dq_i}{dt}) = \frac{d}{dt}(\delta q_i) \\
\therefore \delta A &= \int_{t_1}^{t_2} \sum_i [\frac{\partial L}{\partial q_i} - \frac{d}{dt}(\frac{\partial L}{\partial \dot{q}_i})] \delta q_i dt = 0 \\
& \qquad (\delta q_i : \text{arbitrary})
\end{aligned}$$

$$\therefore \frac{\partial L}{\partial q_i} - \frac{d}{dt}(\frac{\partial L}{\partial q_i}) = 0 : \text{ Lagrange's Equation of Motion} \qquad (2.5)$$

$$\downarrow$$

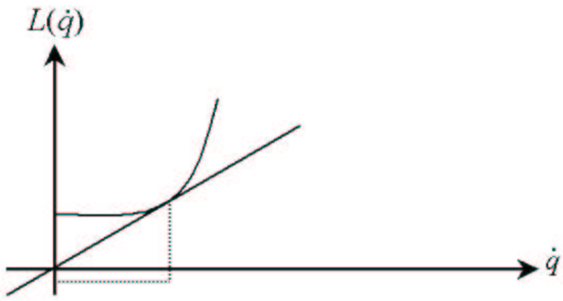
$$\ddot{x} + \omega_0^2 x = 0 \qquad (2.6)$$

2.3 Hamiltonian Mechanics



$$
\begin{aligned}
L &= L(q, \dot{q}; t) \\
&\downarrow \text{ Legendre transformation (tangent transformation)} \\
H &= H(q, p; t)
\end{aligned}
$$

$$(\dot{q} \leftrightarrow p, L \leftrightarrow H)$$



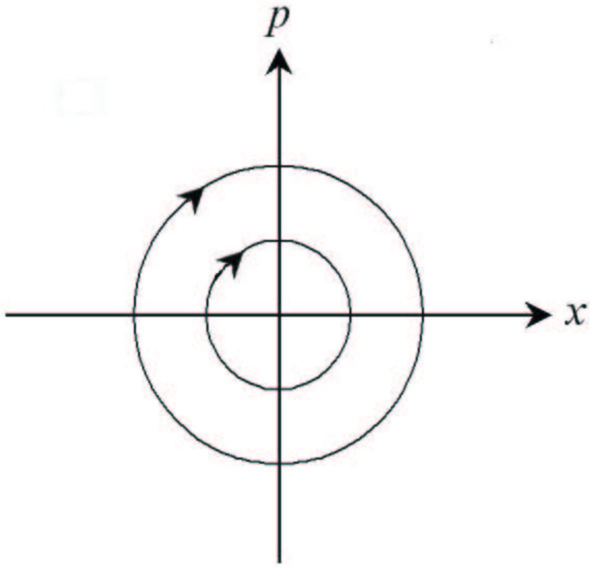
$$\text{Slope} : \frac{\partial L}{\partial \dot{g}} = p$$

$$\text{Intercept} = -H$$

$$p = \frac{L - (-H)}{\dot{q}} \tag{2.7}$$

$$\begin{aligned}\therefore H(q,p) &= p\dot{q} - L, \ \ p = \frac{\partial L}{\partial \dot{q}} \rightarrow \dot{q} = \dot{q}(q,p) \\ &= p\dot{q}(q,p) - L \end{aligned} \tag{2.8}$$

$$\text{S. H. O.} \rightarrow p = \frac{\partial L}{\partial \dot{x}} = m\dot{x} \tag{2.9}$$



Phase space

$$\begin{aligned}\therefore H &= p\dot{x} - \frac{1}{2}m\dot{x}^2 + \frac{1}{2}kx^2 \\ &= \frac{p^2}{2m} + \frac{1}{2}kx^2 \end{aligned} \tag{2.10}$$

$$\delta \int_{t_1}^{t_2} L(q,\dot{q};t)dt = 0 \longrightarrow \delta \int_{t_1}^{t_2} [\vec{p} \cdot \dot{\vec{q}} - H(\vec{q},\vec{p};t)]dt \tag{2.11}$$

$$= \int_{t_1}^{t_2} [(\dot{\vec{q}} - \frac{\partial H}{\partial \vec{p}}) \cdot \delta\vec{p} - (\dot{\vec{p}} + \frac{\partial H}{\partial \vec{q}})\delta\vec{q}\,]dt = 0 \tag{2.12}$$

$$\therefore \dot{\vec{q}} = \frac{\partial H}{\partial \vec{p}}\ , \quad \dot{\vec{p}} = -\frac{\partial H}{\partial \vec{q}} : \text{Hamilton's canonical Eq. of Motion} \tag{2.13}$$

$$\dot{x} = \frac{\partial H}{\partial p} = \frac{p}{m}, \quad \dot{p} = -\frac{\partial H}{\partial x} = -kx \tag{2.14}$$

$$\longrightarrow \quad \ddot{x} = \frac{\dot{p}}{m} = -\omega_0^2 x \tag{2.15}$$

$$\longrightarrow \quad \ddot{x} + \omega_0^2 x = 0 \tag{2.16}$$

2.4 Quantum States

Consider a system with f degrees of freedom. The system can then be described by a wave function $\psi(q_1, \cdots, q_f)$ which is a function of f coordinates required to characterize the system.

A particular quantum state of the system is specified by giving the values of f quantum numbers.

e.g.1

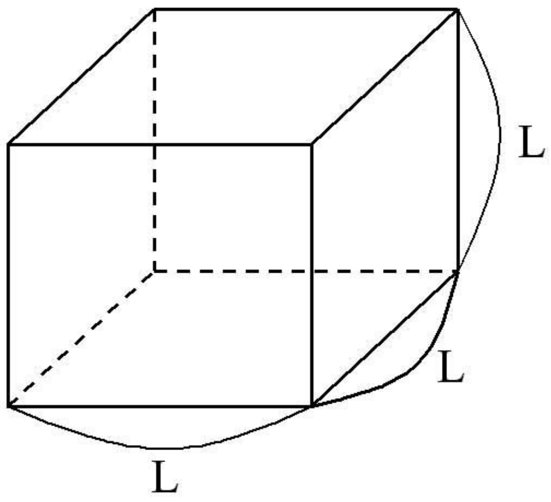
Consider a system of N localized particles, but each having spin $\frac{1}{2}$. The state of the entire system is then specified by stating the values of the N quantum numbers $m_1, \cdots, m_N$ which specify the orientation of the spin of each particle.

$$m_i = \pm\frac{1}{2}, \quad i = 1, \cdots, N. \ \ (m_1, \cdots, m_N) \tag{2.17}$$

e.g.2

Consider a system consisting of N non-interacting particle without spin in a box :

$$\begin{aligned} H = \sum_{i=1}^{N} h_i, \ h_i &= \frac{\vec{p}_i^{\,2}}{2m}, \text{ Stationary state } \ H \cdot \psi = E \cdot \psi \\ \psi(\vec{r}_1, \cdots, \vec{r}_N) &= \prod_{i=1}^{N} \varphi(\vec{r}_i), \quad \vec{r}_i = (x_i, y_i, z_i) \\ h_i \varphi(\vec{r}_i) &= e_i \varphi(\vec{r}_i), \quad E = \sum_{i=1}^{N} e_i \end{aligned}$$



$$
\begin{aligned}
-\frac{\hbar^2}{2m}(\frac{\partial^2}{\partial x^i_2} + \frac{\partial^2}{\partial y^i_2} + \frac{\partial^2}{\partial z^i_2})\varphi &= e_i\varphi \\
\varphi(\vec{r}_i) &= \sin(\pi \cdot \frac{n_{x_i}x_i}{L})\sin(\pi \cdot \frac{n_{y_i}y_i}{L})\sin(\pi \cdot \frac{n_{z_i}z_i}{L}) \\
e_i &= \frac{\hbar^2\pi^2}{2mL^2}(n^2_{x_i} + n^2_{y_i} + n^2_{z_i}) \qquad (2.18)
\end{aligned}
$$

quantum numbers : $\{(n_{x_i}, n_{y_i}, n_{z_i}); i = 1, \cdots, N\}$

e.g.3

Consider a system of three localized particles with spin $\frac{1}{2}$. It is placed in an external constant magnetic field $\vec{B} = B\widehat{z}$

$$H = \sum_{i=1}^{3} h_i, \quad h_i = -\vec{\mu}_i \cdot \vec{B} \qquad (2.19)$$

the set of quantum numbers : (m_1, m_2, m_3)

State index r	Quantum numbers (m_1, m_2, m_3)	Total magnetic moment	Total energy
1	$+++$	3μ	$-3\mu H$
2	$++-$	μ	$-\mu H$
3	$+-+$	μ	$-\mu H$
4	$-++$	μ	$-\mu H$
5	$+--$	$-\mu$	μH
6	$-+-$	$-\mu$	μH
7	$--+$	$-\mu$	μH
8	$---$	-3μ	$3\mu H$

E(total energy) $= -\mu H$: the only information available. (macroscopic condition)

$$\text{Accessible states}: (++-), (+-+), (-++)$$

◦ **Classical approximation**

e. g. a single particle in one dimension The phase space is subdivided into equal cells of area $\delta_p \cdot \delta_q = h_0$