Mecanics using Lagrange and Hamilton approaches

(1) A mechanical system of n particles is described by Newton's law (for $j = 1, 2, \ldots, n$)

$$m_j \frac{d^2 x_j}{dt^2} = \underbrace{- \frac{\partial U(x_1, \ldots, x_n)}{\partial x_j}}_{\text{Force on particle } k} \qquad (I)$$

$U(x_1, \ldots, x_n) =$ Potential energy of the system of n particles.

Show that for $n = 2$ and an elastic potential energy $U(x_1, x_2) = \frac{1}{2} k_1 x_1^2 + \frac{1}{2} k_2 x_2^2$ the laws of motion (I) are identical with

$$\text{(Lagrange)} \qquad \frac{d}{dt} \frac{\partial \mathcal{L}}{\partial \dot{x}_j} - \frac{\partial \mathcal{L}}{\partial x_j} = 0 \qquad j = 1, 2$$

for

$$\mathcal{L}(x_1, x_2, \dot{x}_1, \dot{x}_2) = \frac{1}{2} m_1 \dot{x}_1 + \frac{1}{2} m_2 \dot{x}_2 - U(x_1, x_2)$$

(2) Show that the same equations (I) are identical with

$$\dot{q}_j = \frac{\partial H}{\partial p_j}$$

$$\dot{p}_j = -\frac{\partial H}{\partial q_j}$$

(Hamilton)

where $H(p_1, p_2, q_1, q_2) = \frac{p_1^2}{2\mu_1} + \frac{p_2^2}{2\mu_2} + U(q_1, q_2)$

with

$q_1 = x_1$

$q_2 = x_2$

$p_1 = \mu_1 \dot{x}_1$

$q_1 = \mu_2 \dot{x}_2$

(3) Show that you can obtain the Lagrangian $\mathcal{L}$ from the Hamiltonian H as follows

(1) Given p_1 and p_2, solve for $\dot{q}_1$ and $\dot{q}_2$ from

$$p_1 = \frac{\partial \mathcal{L}}{\partial \dot{q}_1}$$

$$p_2 = \frac{\partial \mathcal{L}}{\partial \dot{q}_2}$$

(2) Insert $\dot{q}_1$ and $\dot{q}_2$ from (1) into

$$H = p_1 \dot{q}_1 + p_2 \dot{q}_2 - \mathcal{L}(q_1, q_2, \dot{q}_1, \dot{q}_2)$$

Quantum mechanics

The classical Hamiltonian of a free particle
the potential energy $= 0$

is $H(p_x, p_y, p_z) = \frac{p_x^2}{2m} + \frac{p_y^2}{2m} + \frac{p_z^2}{2m}$

In quantum mechanics you need to change p_x, p_y, and p_z into

$$p_x \rightarrow \frac{\hbar}{i}\frac{\partial}{\partial x}$$

$$p_y \rightarrow \frac{\hbar}{i}\frac{\partial}{\partial y}$$

$$p_z \rightarrow \frac{\hbar}{i}\frac{\partial}{\partial z}$$

and get the quantum Hamiltonian

$$H = -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right)$$

To find the quantum probabilities you need to find a function

$$\psi(x, y, z, t)$$

such that

$$i\hbar \frac{\partial \psi}{\partial t} = H \psi$$

that is

(Schroedinger) $$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m}\left(\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} + \frac{\partial^2 \psi}{\partial z^2} \right)$$

1. Put $$\psi(x,y,z,t) = \varphi(x,y,z)\, e^{-\frac{i}{\hbar}Et}$$

in Schroedinger equation and show that

$$\frac{\partial^2 \varphi}{\partial x^2} + \frac{\partial^2 \varphi}{\partial y^2} + \frac{\partial^2 \varphi}{\partial z^2} + \frac{2mE}{\hbar^2}\varphi = 0 \qquad (\mathrm{II})$$

2. Insert in (II) a $\varphi(x,y,z)$ of the form

$$\varphi(x,y,z) = A\, e^{i(k_1 x + k_2 y + k_3 z)}$$

and show that

$$E = \frac{\hbar^2}{2m}\left(k_1^2 + k_2^2 + k_3^2\right)$$

3. Show that

$$\frac{\hbar}{i}\frac{\partial}{\partial x}\varphi = \hbar k_1 \varphi \,;\; \frac{\hbar}{i}\frac{\partial}{\partial y}\varphi = \hbar k_2 \varphi \,;\; \frac{\hbar}{i}\frac{\partial}{\partial z}\varphi = \hbar k_3 \varphi$$

(4) Boundary condition. Now $\psi(x, y, z)$ is periodic with spatial period (L_x, L_2, L_3)

$$\begin{cases} \psi(x+L_1, y, z) = \psi(x, y, z) \\ \psi(x, y+L_2, z) = \psi(x, y, z) \\ \psi(x, y, z+L_3) = \psi(x, y, z) \end{cases} \qquad (\overline{\underline{III}})$$

Show that to satisfy $(\overline{\underline{III}})$ one must require that

$$k_1 = \frac{2\pi}{L_1} n_1 \quad ; \quad n_1 = 0, \pm 1, \pm 2, \ldots$$

$$k_2 = \frac{2\pi}{L_2} n_2 \quad ; \quad n_2 = 0, \pm 1, \pm 2, \ldots$$

$$k_3 = \frac{2\pi}{L_3} n_3 \quad ; \quad n_3 = 0, \pm 1, \pm 2, \ldots$$

(5) Express E in (2) in terms of n_1, n_2 and n_3.