PHYS 3803: Quantum Mechanics I, Spring 2021

Lecture 2, January 28, 2021 (Thursday)

- Midterm Exam: March 16 (Tuesday), 1:00 p.m.–3:00 p.m.
- Reading: Mathematical Tools (Chapter 3 in Griffiths)
- Assignment: Problem Set 1 due February 03 (Wednesday).
  Make a pdf file and send it to our grader: jmderkacy@ou.edu

Topics for Today: Review of Classical Mechanics

1.6 The Hamiltonian Dynamics

1.7 The Hamiltonian and Energy

1.8 Poisson Brackets and Hamilton Equations

1.9 Quantum Correspondence Principle

Topics for Next Lecture: Mathematical Tools

2.1 Linear Vector Spaces

2.2 Inner Product and Inner Product Spaces

2.3 Dirac Notation

2.4 Linear Operators

2.5 Eigenvectors and Eigenvalues

1.6 The Hamiltonian Dynamics

Recall that $T(q, \dot{q}, t) =$ the kinetic energy, $U(q, \dot{q}, t) =$ the potential energy, and the Lagrangian is defined as

$$L(q, \dot{q}, t) \equiv T(q, \dot{q}, t) - U(q, \dot{q}, t) \,.$$

With the conjugate momentum $p_i \equiv \partial L / \partial \dot{q}_i$, the Legendre transformation takes $L(q_i, \dot{q}_i, t)$ to $H(q_i, \partial L / \partial \dot{q}_i, t) = H(q_i, p_i, t)$.

The Hamiltonian is defined as

$$H(q, p, t) \equiv \sum_i \dot{q}_i \left(\frac{\partial L}{\partial \dot{q}_i} \right) - L(q, \dot{q}, t) = \sum_i \dot{q}_i p_i - L(q, \dot{q}, t) \,.$$

Applying the Euler-Lagrange equation, we obtain

$$dH = d\left[\sum_i \dot{q}_i p_i - L(q,\dot{q},t)\right] = \sum_i \left[\dot{q}_i dp_i - \dot{p}_i dq_i\right] - \frac{\partial L}{\partial t} dt\,.$$

with $\dot{p}_i = (d/dt)(\partial L/\partial \dot{q}_i) = \partial L/\partial q_i$.

On the other hand, the total differential of $H = H(q,p,t)$ is

$$\begin{aligned} dH(q,p,t) &= \sum_i \left(\frac{\partial H}{\partial q_i} dq_i + \frac{\partial H}{\partial p_i} dp_i\right) + \frac{\partial H}{\partial t} dt \\ &= \sum_i \left(-\dot{p}_i dq_i + \dot{q}_i dp_i\right) - \frac{\partial L}{\partial t} dt\,. \end{aligned}$$

Identifying the coefficients of dq_i, dp_i, and dt, we obtain $\partial H/\partial t = -\partial L/\partial t$, and Hamilton equations of motion

$$\dot{q}_i = +\frac{\partial H}{\partial p_i}\,, \quad \text{and} \quad \dot{p}_i = -\frac{\partial H}{\partial q_i}\,,$$

which are also called the canonical equations of motion.

Example 1:

Let us consider a particle of mass m constrained to move on the surface of a cylinder defined by $x^2 + y^2 = R^2 = \text{constant}$. This particle is subject to a force

$$\vec{F} = -k\vec{r} = -kr\hat{r}\,.$$

With $R = \text{constant}$, $\dot{R} = 0$, the kinetic energy is

$$T = \frac{1}{2}m(\dot{x}^2 + \dot{y}^2 + \dot{z}^2) = \frac{1}{2}m(R^2\dot{\phi}^2 + \dot{z}^2)\,.$$

The potential energy is

$$\begin{aligned} U(r) &= -\int_0^r \vec{F}(\vec{s}) \cdot d\vec{s} \\ &= \frac{1}{2}kr^2 = \frac{1}{2}k(R^2 + z^2)\,, \end{aligned}$$

where we have applied $\hat{r} \cdot d\hat{r} = 0$, since $\hat{r} \cdot \hat{r} = 1$.

The Lagrangian can be expressed as

$$\begin{aligned} L &= T - U \\ &= \frac{1}{2}m(R^2\dot{\phi}^2 + \dot{z}^2) - \frac{1}{2}k(R^2 + z^2). \end{aligned}$$

The generalized coordinates are ϕ and z for a cylinder with $R =$ constant, and the generalized momenta are

$$p_\phi = \frac{\partial L}{\partial \dot{\phi}} = mR^2\dot{\phi},$$

and

$$p_z = \frac{\partial L}{\partial \dot{z}} = m\dot{z}.$$

Applying the expressions for the generalized momenta, we have

$$\begin{aligned} \dot{\phi} &= \frac{p_\phi}{mR^2}, \quad \text{and} \\ \dot{z} &= \frac{p_z}{m}. \end{aligned}$$

The Hamiltonian is

$$\begin{aligned}
H(\phi, p_\phi, z, p_z) &= \dot{\phi} p_\phi + \dot{z} p_z - L(\phi, \dot{\phi}, z, \dot{z}) \\
&= \dot{\phi} p_\phi + \dot{z} p_z - \left[\frac{1}{2} m R^2 \dot{\phi}^2 + \frac{1}{2} m \dot{z}^2 - \frac{1}{2} k (R^2 + z^2)\right] \\
&= \frac{p_\phi}{mR^2} p_\phi + \frac{p_z}{m} p_z \\
&\quad - \left[\frac{1}{2} m R^2 \left(\frac{p_\phi}{mR^2}\right)^2 + \frac{1}{2} m \left(\frac{p_z}{m}\right)^2 - \frac{1}{2} k (R^2 + z^2)\right] \\
&= \frac{p_\phi^2}{2mR^2} + \frac{p_z^2}{2m} + \frac{1}{2} k (R^2 + z^2).
\end{aligned}$$

The Hamilton equations of motion are

$$\begin{aligned}
\dot{p}_\phi &= -\frac{\partial H}{\partial \phi} = 0\,, \quad \text{and} \quad \dot{\phi} = \frac{\partial H}{\partial p_\phi} = \frac{p_\phi}{mR^2}\,, \\
\dot{p}_z &= -\frac{\partial H}{\partial z} = -kz\,, \quad \text{and} \quad \dot{z} = \frac{\partial H}{\partial p_z} = \frac{p_z}{m}\,.
\end{aligned}$$

Combining

$$\dot{p}_z = -\frac{\partial H}{\partial z} = -kz, \, , \quad \text{and} \quad \dot{z} = \frac{\partial H}{\partial p_z} = \frac{p_z}{m} \, ,$$

we obtain

$$\ddot{z} = \frac{\dot{p}_z}{m} = -(k/m)z,$$

i.e.

$$\ddot{z} + \omega_0^2 z = 0,$$

where $\omega_0 = \sqrt{k/m}$.

Note that

(a). For $T = T(q, \dot{q})$ and $U = V(q)$, the Hamiltonian $H = T + U = E$.

(b). In this example, $\dot{p}_\phi = -\partial H/\partial \phi = 0$, then $p_\phi = mR^2\dot{\phi} =$ constant.

(c). The motion of the particle in the z direction is simple harmonic.

1.7 The Hamiltonian and Energy

For a system with generalized coordinates q_i, the Lagrangian is

$$L = L(q_i, \dot{q}_i, t)\,, \quad i = 1, 2, \cdots, N\,,$$

and the Hamiltonian is

$$H \equiv \sum_{i=1}^{N} \dot{q}_i \frac{\partial L}{\partial \dot{q}_i} - L(q, \dot{q}, t) = \sum_{i=1}^{N} \dot{q}_i p_i - L(q, \dot{q}, t)\,,$$

where q is a vector.

The time derivative of the Hamiltonian is

$$\frac{d}{dt}H = \frac{d}{dt}\left[\sum_{i=1}^{N}\dot{q}_i p_i - L(q,\dot{q},t)\right]$$

$$= \sum_{i=1}^{N}\left(\ddot{q}_i p_i + \dot{q}_i \frac{d}{dt}\frac{\partial L}{\partial \dot{q}_i}\right) - \left[\sum_{i=1}^{N}\left(\frac{\partial L}{\partial q_i}\dot{q}_i + \frac{\partial L}{\partial \dot{q}_i}\ddot{q}_i\right) + \frac{\partial L}{\partial t}\right].$$

Applying Euler-Lagrange equations $\partial L/\partial q_i - d/dt(\partial L/\partial \dot{q}_i) = 0$, we obtain

$$\frac{dH}{dt} = -\frac{\partial L}{\partial t}.$$

If the Lagrangian L does not depend on time explicitly, then the Hamiltonian is a constant of the trajectory.
If $dH/dt = 0$ then $H =$ constant.

Exercise: Find the Hamiltonian $H(p,x)$ with the Lagrangian $L = (1/2)m\dot{x}^2 - U(x)$.

For a Lagrangian of the form

$$L(x, \dot{x}) = \frac{1}{2}m\dot{x}^2 - U(x),$$

the conjugate momentum is

$$p = \frac{\partial L}{\partial \dot{x}} = m\dot{x}, \quad \dot{x} = \frac{p}{m},$$

and the Hamiltonian is

$$\begin{aligned} H &= \dot{x}p - L(x, \dot{x}) \\ &= \dot{x}p - \left[\frac{1}{2}m\dot{x}^2 - U(x)\right] \\ &= \left(\frac{p}{m}\right)p - \frac{1}{2}m\left(\frac{p}{m}\right)^2 + U(x) \\ &= \frac{p^2}{2m} + U(x), \end{aligned}$$

which is the energy $E = T + U$.

1.8 Poisson Brackets and Hamilton Equations

Poisson brackets provide a formal way to get the quantum mechanical commutation relation for systems that can be described classically.

Let us consider classical observables A(p,q,t) and B(p,q,t) that are functions of the coordinates, the momenta, and perhaps time. The **Poisson bracket** between two observables is defined as

$$\{A, B\} \equiv \sum_{i=1}^{N} \left(\frac{\partial A}{\partial q_i} \frac{\partial B}{\partial p_i} - \frac{\partial A}{\partial p_i} \frac{\partial B}{\partial q_i} \right) .$$

The Poisson bracket product is like vector cross products and matrix commutators, satisfies the anticommutativity

$$\{B, A\} = -\{A, B\} ,$$

and the Jacobi identity

$$\{\{A, B\}, C\} + \{\{C, A\}, B\} + \{\{B, C\}, A\} = 0 .$$

Here are some important relations:

$$\{q_i, q_j\} = 0 = \{p_i, p_j\}\,, \quad \text{and} \quad \{q_i, p_j\} = \delta_{ij} = -\{p_i, q_j\}\,,$$

where δ_{ij} is the Kronecker's δ symbol.

Furthermore, we recognize conserved quantities quite easily in the Hamiltonian formalism. Let's consider an observable ω as $\omega(q, p)$. We can show that

$$\frac{d\omega}{dt} = \{\omega, H\} + \frac{\partial \omega}{\partial t}\,, \quad \text{(Homework)}\;.$$

For $\partial\omega/\partial t = 0$, we have

$$\frac{d\omega}{dt} = 0, \;\; \text{if} \;\; \{\omega, H\} = 0.$$

Since $\{H, H\} = 0$, this shows that the Hamiltonian of the total energy of the system is a constant in time.

1.9 Quantum Correspondence Principle

The commutation relation of two operators A and B is defined as

$$[A, B] \equiv AB - BA\,.$$

Quantum commutators satisfy the following relations:

(i) $[A, B] = -[B, A]$

(ii) $[A + B, C] = [A, C] + [B, C]$

(iii) $[AB, C] = A[B, C] + [A, C]B$

(iv) $[A, BC] = B[A, C] + [A, B]C$

Exercise: Let us consider X, P, and H as quantum operators, find

- (a) $[X, P^2]$, and
- (b) $[X, H]$, with

$$H = \frac{P^2}{2m} + V(X)\,.$$