SPA5304 Physical Dynamics Lecture 26-27

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1 Hamiltonian mechanics

1.1 Example: Particle in a potential $V(\vec{r})$

$$L = \frac{m}{2}\dot{\vec{r}}^2 - V(\vec{r})$$

$$\vec{p} = \frac{\partial L}{\partial \dot{\vec{r}}} = m\dot{\vec{r}}$$

We need to express $\dot{\vec{r}} = \dot{\vec{r}}(\vec{r}, \vec{p}, t)$. We get

$$\dot{\vec{r}} = \frac{\vec{p}}{m}$$

$$H = \vec{p}\cdot\dot{\vec{r}} - L = \vec{p}\cdot\frac{\vec{p}}{m} - \left(\frac{1}{2}m\left(\frac{\vec{p}}{m}\right)^2 - V(\vec{r})\right) = \frac{\vec{p}^2}{2m} + V(\vec{r})$$

Hamilton's equations:

$$\begin{cases} \dot{\vec{r}} = \frac{\partial H}{\partial \vec{p}} = \frac{\vec{p}}{m} \\ \\ \dot{\vec{p}} = -\frac{\partial H}{\partial \vec{r}} = -\frac{\partial V}{\partial \vec{r}} \end{cases}$$

In particular, for the free particle ($V = 0$), $\vec{r}$ is cyclic $\Rightarrow \dot{\vec{p}} = 0 \Rightarrow \vec{p}$ is constant.

1.2 Example: Particle in a central potential in polar coordinates

$$L = \frac{m}{2}(\dot{r}^2 + r^2\dot{\phi}^2) - V(\vec{r})$$

$$p_r = \frac{\partial L}{\partial \dot{r}} = m\dot{r} \qquad p_\phi = \frac{\partial L}{\partial \dot{\phi}} = mr^2\dot{\phi}$$

$$H = p_r\dot{r} + p_\phi\dot{\phi} - L = p_r\frac{p_r}{m} + p_\phi\frac{p_\phi}{mr^2} - \frac{m}{2}\left(\left(\frac{p_r}{m}\right)^2 + r^2\left(\frac{p_\phi}{mr^2}\right)^2\right) + V(r)$$

$$\boxed{H = \frac{p_r^2}{2m} + \frac{p_\phi^2}{2mr^2} + V(r)}$$

Hamilton's equations for r:

$$\begin{cases} \dot{r} = \frac{\partial H}{\partial p_r} = \frac{p_r}{m} \\ \\ \dot{p}_r = -\frac{\partial H}{\partial r} = \frac{p_\phi^2}{mr^3} - V'(r) = -\frac{\partial}{\partial r}\underbrace{\left[V(r) + \frac{p_\phi^2}{2mr^2}\right]}_{V_{\text{eff}}(r)} \end{cases}$$

and for ϕ:

$$\begin{cases} \dot{\phi} = \frac{\partial H}{\partial p_\phi} = \frac{p_\phi}{mr^2} \\ \\ \dot{p}_\phi = -\frac{\partial H}{\partial \phi} = 0 \qquad \Rightarrow \qquad p_\phi = mr^2\dot{\phi} = \text{const.} \end{cases}$$

1.3 Time evolution in Hamiltonian mechanics

$$A = A(\vec{q},\, \vec{p},\, t) : \quad \text{Some physical quantity of the system.}$$

How does it evolve?

$$\dot{A} = \frac{dA}{dt} = \frac{\partial A}{\partial q_i}\dot{q}_i + \frac{\partial A}{\partial p_i}\dot{p}_i + \frac{\partial A}{\partial t}$$

Using Hamilton's equations this is

$$\dot{A} = \frac{\partial A}{\partial q_i}\frac{\partial H}{\partial p_i} - \frac{\partial A}{\partial p_i}\frac{\partial H}{\partial q_i} + \frac{\partial A}{\partial t}$$

If we define the **Poisson bracket** by

$$\boxed{\{X,\, Y\} \equiv \frac{\partial X}{\partial q_i}\frac{\partial Y}{\partial p_i} - \frac{\partial X}{\partial p_i}\frac{\partial Y}{\partial q_i}}$$

then

$$\boxed{\dot{A} = \{A,\, H\} + \frac{\partial A}{\partial t}}$$

1.4 Aside: Poisson brackets and quantum mechanics

There is a special $\{,\}$, namely:

$$\{x,\, p\} = \frac{\partial x}{\partial x}\frac{\partial p}{\partial p} - \frac{\partial x}{\partial p}\frac{\partial p}{\partial x} = 1$$

The **canonical commutation relation** of quantum mechanics is

$$[\hat{x},\, \hat{p}] \equiv \hat{x}\hat{p} - \hat{p}\hat{x} = i\hbar$$

(In the basis where the operator $\hat{x}$ means multiplying the wavefunction by x, while $\hat{p}$ is nothing but the derivative: $\hat{p} = -i\hbar\frac{\partial}{\partial x}$.)

The similarity between the Poisson bracket and the commutator suggests that we can go from classical mechanics to quantum mechanics by replacing

$$\{X,\, Y\} \to \frac{1}{i\hbar}[\hat{X},\, \hat{Y}]$$

where the hatted quantities are operators.

Using this "dictionary" (whenever it works), the time evolution of a quantum mechanical operator $\hat{A}$ should be

$$\dot{\hat{A}} = \frac{1}{i\hbar}[\hat{X},\, \hat{H}] + \frac{\partial \hat{A}}{\partial t}$$

This is the so-called Heisenberg equation in quantum mechanics.

1.5 Properties of Poisson brackets

(i)
$$\{A,\, B\} = -\{B,\, A\}$$

(ii)
$$\{A,\, A\} = 0$$

(iii)
$$\{A,\, c\} = 0$$

if $c =$const.

(iv)
$$\{A + B,\, C\} = \{A,\, C\} + \{B,\, C\}$$

(v)
$$\{A,\, BC\} = B\{A,\, C\} + \{A,\, B\}C$$

(vi) The Jacobi identity
$$\{A,\, \{B,\, C\}\} + \{B,\, \{C,\, A\}\} + \{C,\, \{A,\, B\}\} = 0$$

1.6 A consequence of the Jacobi identity

If $\dot{I}_1 = \dot{I}_2 = 0$, i.e. they are both conserved, then $\{I_1, I_2\}$ is also conserved (Poisson's theorem). This way we can generate a new conserved quantity (unless it is just a combination of the old I_1 and I_2).

Proof:

$$\frac{d}{dt}\{I_1, I_2\} = \{\{I_1, I_2\}, H\} + \frac{\partial}{\partial t}\{I_1, I_2\}$$

using the Jacobi identity we get

$$= -\{\{I_2, H\}, I_1\} - \{\{H, I_1\}, I_2\} + \{\frac{\partial I_1}{\partial t}, I_2\} + \{I_1, \frac{\partial I_2}{\partial t}\}$$

$$= \left\{-\{I_2, H\} - \frac{\partial I_2}{\partial t},\, I_1\right\} + \left\{-\{H, I_1\} + \frac{\partial I_1}{\partial t},\, I_2\right\} = 0$$

Q.E.D.

1.7 A charged particle in an electromagnetic field

The Lagrangian of a particle of mass m and charge e in an external electromagnetic field is

$$\boxed{L = \frac{1}{2}m\dot{\vec{r}}^2 - V(\vec{r}, \dot{\vec{r}})}$$

with

$$\boxed{V(\vec{r}, \dot{\vec{r}}) = e\phi - e\dot{\vec{r}} \cdot \vec{A}}$$

where $\phi(\vec{r}, t)$ and $\vec{A}(\vec{r}, t)$ are the scalar and vector potentials related to electromagnetic fields $\vec{E}$ and $\vec{B}$ via

$$\boxed{\vec{E} = -\partial_t \vec{A} - \vec{\nabla}\phi}$$

$$\boxed{\vec{B} = \vec{\nabla} \times \vec{A}}$$

(This is our first encounter with a velocity-dependent potential. In this case, force is not given by $-\frac{\partial V}{\partial q}$; see Goldstein §1.5)

We prove the above by showing that the Euler-Lagrange equation derived from the above Lagrangian is the familiar

$$\boxed{m\ddot{x}_i = eE_i + e(\dot{\vec{r}} \times \vec{B})_i}$$

where $i = 1, 2, 3$. Note that we have set $c = 1$.

Proof:

$$L = \frac{1}{2} m \dot{\vec{r}}^2 - e\phi + e\dot{\vec{r}} \cdot \vec{A}$$

$$p_i = \frac{\partial L}{\partial \dot{x}_i} = m\dot{x}_i + eA_i$$

$$\frac{\partial L}{\partial x_i} = -e\nabla_i \phi + e\dot{x}_j \nabla_i A_j$$

$$\dot{p}_i = m\ddot{x}_i + e\frac{d}{dt} A_i(\vec{r}, t) = m\ddot{x}_i + e(\partial_t A_i + \dot{x}_j \nabla_j A_i)$$

So the Euler-Lagrange equations ($\dot{p}_i = \frac{\partial L}{\partial x_i}$) give

$$m\ddot{x}_i + e(\partial_t A_i + \dot{x}_j \nabla_j A_i) = -e\nabla_i \phi + e\dot{x}_j \nabla_i A_j$$

$$m\ddot{x}_i = e\underbrace{(-\partial_t A_i - \nabla_i \phi)}_{E_i} + e\dot{x}_j(\nabla_i A_j - \nabla_j A_i)$$

But

$$(\dot{\vec{r}} \times \vec{B})_i = (\dot{\vec{r}} \times (\vec{\nabla} \times \vec{A}))_i = \epsilon_{ijk} \dot{x}_j (\vec{\nabla} \times \vec{A})_k = \epsilon_{ijk} \dot{x}_j \epsilon_{klm} \nabla_l A_m$$

Using the identity: $\epsilon_{kij}\epsilon_{klm} = \delta_{il}\delta_{jm} - \delta_{im}\delta_{jl}$ we get

$$(\delta_{il}\delta_{jm} - \delta_{im}\delta_{jl}) \dot{x}_j \nabla_l A_m = \dot{x}_j (\nabla_i A_j - \nabla_j A_i)$$

Therefore,

$$m\ddot{x}_i = eE_i + e(\dot{\vec{r}} \times \vec{B})_i$$

Q.E.D.

1.8 Remark 1: Lorentz invariance

The interaction term

$$S_{\text{int}} = -\int dt\, V = -\int dt (e\phi - e\dot{\vec{r}} \cdot \vec{A})$$

can be written as

$$\boxed{S_{\text{int}} = -\int d^4x (\rho\phi - \vec{J} \cdot \vec{A}) = \int d^4x\, J^\mu A_\mu}$$

where

$$\boxed{A_\mu = (-\phi,\, \vec{A})}$$

$$\boxed{J^\mu = (\rho,\, \vec{J})}$$

These are **four-vectors** of relativity. ρ is the charge density and $\vec{J}$ is the current density.

In the above point-particle case:

$$\boxed{\rho = e\delta^{(3)}(\vec{r} - \vec{r}(t))}$$

$$\boxed{\vec{J} = e\dot{\vec{r}}\delta^{(3)}(\vec{r} - \vec{r}(t))}$$

where the particle of charge e is moving along the trajectory $\vec{r} = \vec{r}(t)$.

$J^\mu A_\mu$ is a scalar (invariant under Lorentz transformations), so the action is also Lorentz invariant.

1.9 Remark 2: "gauge invariance"

We have previously seen that the Euler-Lagrange equations are unchanged if the Lagrangian is changed by a total derivative.

We have

$$L = \frac{1}{2}m\dot{\vec{r}}^2 + L_{\text{int}}$$

$$L_{\text{int}} = -e\phi + e\dot{\vec{r}} \cdot \vec{A}$$

Let us consider the transformation

$$A_\mu \to A_\mu + \partial_\mu \Lambda$$

Here we used the notation $\partial_\mu \equiv (\partial_t, \vec{\nabla})$ and $\mu = 0, 1, 2, 3$. Here $\Lambda = \Lambda(\vec{r}, t)$ is an arbitrary function. The above transformation means

$$\phi \to \phi - \partial_t \Lambda$$

and

$$\vec{A} \to \vec{A} + \vec{\nabla}\Lambda$$

It is a **gauge transformation**.

$$L_{\text{int}} \to L'_{\text{int}} = L_{\text{int}} + e\partial_t \Lambda + e\dot{\vec{r}} \cdot \vec{\nabla}\Lambda = L_{\text{int}} + e\frac{d}{dt}\Lambda(\vec{r}(t), t)$$

The second term is a total derivative and thus it will not affect the Euler-Lagrange equations. Hence, the transformation is a symmetry of the theory[1] and this is called **gauge invariance**.

• One can understand this also by noting that the physical fields $\vec{E}, \vec{B}$ do not change under gauge transformations:

$$\vec{E} = -\partial_t \vec{A} - \vec{\nabla}\phi \quad \to \quad -\partial_t \underbrace{(\vec{A} + \vec{\nabla}\Lambda)}_{\vec{A}'} - \vec{\nabla} \underbrace{(\phi - \partial_t \Lambda)}_{\phi'} = \vec{E}$$

and

$$\vec{B} = \vec{\nabla} \times \vec{A} \quad \to \quad \vec{\nabla} \times (\vec{A} + \vec{\nabla}\Lambda) = \vec{\nabla} \times \vec{A} + \underbrace{\vec{\nabla} \times \vec{\nabla}\Lambda}_{0} = \vec{B}$$

[1] It really is not a physical symmetry, but a redundancy in the description of the physical degrees of freedom.

• There are infinitely many different ways to choose $(\phi, \vec{A})$ that give the same $\vec{E}, \vec{B}$. This arbitrariness can be removed by "fixing the gauge", i.e. by imposing some conditions to be satisfied by ϕ and $\vec{A}$.

For instance the Coulomb (or radiation) gauge is:

$$\vec{\nabla} \cdot \vec{A} = 0$$

Can we do further gauge transformations while staying in this gauge?

$$0 = \vec{\nabla} \cdot \vec{A}' = \vec{\nabla} \cdot (\vec{A} + \vec{\nabla}\Lambda) = \nabla^2 \Lambda = 0$$

If we require that $\Lambda \to 0$ as $|\vec{r}| \to \infty$, the only solution is $\Lambda = 0$. Thus, the Coulomb gauge choice completely fixes the gauge.

1.10 Hamiltonian of a charged particle

$$L = \frac{1}{2} m \dot{\vec{r}}^2 - e\phi + e\dot{\vec{r}} \cdot \vec{A}$$

$$p_i = \frac{\partial L}{\partial \dot{x}_i} = m\dot{x}_i + eA_i \qquad \Rightarrow \qquad \dot{x}_i = \frac{1}{m}(p_i - eA_i)$$

$$\begin{aligned} H = p_i \dot{x}_i - L &= p_i \frac{1}{m}(p_i - eA_i) - \left[\frac{1}{2} m \frac{1}{m^2}(p_i - eA_i)^2 - e\phi + e\frac{1}{m}(p_i - eA_i)A_i\right] \\ &= (p_i - eA_i)\frac{1}{m}(p_i - eA_i) - \frac{1}{2m}(p_i - eA_i)^2 + e\phi \end{aligned}$$

$$\boxed{H = \frac{1}{2m}(\vec{p} - e\vec{A})^2 + e\phi}$$

• The Hamiltonian of a charged particle is obtained by

(i) Perform "minimal substitution":

$$\vec{p} \to \vec{p} - e\vec{A}$$

(ii) Add the potentia lterm, $e\phi$

1.11 A peek at quantum mechanics

What is the Schroedinger equation for a particle of mass m and charge e in an electromagnetic field?

$$H_{\text{classical}} = \frac{1}{2m}(\vec{p} - e\vec{A})^2 + e\phi$$

In quantum mechanics, $\vec{p} \to -i\hbar\vec{\nabla}$. So

$$(\vec{p} - e\vec{A})^2 \to (-i\hbar\vec{\nabla} - e\vec{A})^2 = -\hbar^2\vec{\nabla}^2 + e^2\vec{A}^2 + i\hbar e(\vec{A}\cdot\vec{\nabla} + \vec{\nabla}\cdot\vec{A}) = -\hbar^2\vec{\nabla}^2 + e^2\vec{A}^2 + 2i\hbar e\vec{A}\cdot\vec{\nabla} + i\hbar e(\vec{\nabla}\cdot\vec{A})$$

If we go to Coulomb gauge, then $\vec{\nabla}\cdot\vec{A} = 0$. So in this gauge the Schroedinger equation is

$$\left(-\frac{\hbar^2}{2m}\vec{\nabla}^2 + \frac{e^2}{2m}\vec{A}^2 + \frac{i\hbar}{m}\vec{A}\cdot\vec{\nabla} + e\phi\right)\Psi = E\Psi$$