Lectures 16 - 21 (13th - 25th of November 2014)

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5 The Hamiltonian Formalism

5.1 Phase Space, Legendre Transform, Hamilton's Equations, the Principle of Least Action

Key concepts: phase space, Hamiltonian, Legendre Transform.

The basic motivation behind Hamiltonian Formalism is to eliminate generalised velocities in favour of generalised momenta and place generalised coordinates and conjugate momenta on equal footing.
We introduced the concept of Phase space and then defined the Hamiltonian to be the Legendre transform of the Lagrangian with respect to generalised velocities $\dot{q}_i$,

$$H(\boldsymbol{q},\boldsymbol{p},t) = p_i\dot{q}_i - L(\boldsymbol{q},\dot{\boldsymbol{q}},t). \tag{1}$$

The recipe for eliminating $\dot{q}_i$ in the RHS is simple: we invert $p_i(\boldsymbol{q},\dot{\boldsymbol{q}},t) = \frac{\partial L}{\partial \dot{q}_i}$ to obtain $\dot{q}_i(\boldsymbol{q},\boldsymbol{p},t)$ and substitue it into (3). Hamiltonian acts on the phase space, i.e. $H = H(\boldsymbol{q},\boldsymbol{p},t)$.

We then derived Hamilton's Equations

$$\begin{aligned} \dot{p}_i &= -\frac{\partial H}{\partial q_i}, \\ \dot{q}_i &= \frac{\partial H}{\partial p_i}. \end{aligned} \tag{2}$$

These are $2n$ 1st order differential equations for q_i and p_i. (Compare with n 2nd order DE for q_i and $\dot{q}_i$ in Lagrangian formalism.) We derived (2) using two methods.

(a) First, by considering the differential of (1). On the one hand,

$$dH = \dot{q}_i dp_i - \frac{\partial L}{\partial q_i}dq_i - \frac{\partial L}{\partial t}dt.$$

On the other hand,

$$dH = \frac{\partial H}{\partial q_i}dq_i + \frac{\partial H}{\partial p_i}dp_i + \frac{\partial H}{\partial t}dt.$$

(b) Second, by varying the action integral,

$$S = \int_{t_1}^{t_2}[p_i\dot{q}_i - H(\boldsymbol{q},\boldsymbol{p},t)]dt.$$

We pointed out that, unlike in Lagrangian formalism where $\dot{q}$ varied authomatically with q, here we have to vary q and p independently. This supports our vision that q and p can be treated equally. However, there is a difference after all. We only have to require that $\delta q_i(t_1) = \delta q_i(t_2) = 0$, while p_i can be free at t_1 and t_2. To restore the symmetry between q and p we can simply impose $\delta p_i(t_1) = \delta p_i(t_2) = 0$. This will have an additional advantage of us being able to add full time derivatives of arbitrary functions $F(q,p)$ to the action inside the integral.

We discuss two conservation laws, namely

(a) If $\frac{\partial H}{\partial t} = 0$ then H is a constant of motion. It follows trivially from $\frac{\partial H}{\partial t} = -\frac{\partial L}{\partial t}$.

(b) If q is ignorable (cyclic) with respect to the Lagrangian, then it is also ignorable w.r.t the Hamiltonian. This follows by construction, indeed $p = \frac{\partial L(\dot{q})}{\partial \dot{q}_i} = p(\dot{q})$, since L does not depend on q.

We consider two examples:

(1) A particle moving in 3-dimensional potential (trivial example)

(2) A charged particle in electro-magnetic field.
We derive the Hamiltonian in the form

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

One can now write Hamilton's equations and verify that they give Lorentz force law. We didn't do it explicitly. We consider a particular case with $\boldsymbol{A} = (-By, 0, 0)$, which corresponds to uniform magnetic field of magnitude B is z-direction. We show that for a particle which moved in (x,y)-plane the motion will be circular.

5.2 Liouville's Theorem

We stated and proved Liouville's theorem: the volume of a region in phase-space is conserved under Hamiltonian time evolution.

We introduce the phase-space density function $\rho(q, p, t)$. This can be interpreted in two different ways. First interpretation is probabilistic: ρdV is the probability that the system will be found in dV. The second is ensemble interpretation: ρdV is the number of particle confined by dV. Since the number of particle in a given co-moving volume is conserved, we can rephrase the Liouville's Theorem as follows.

$$\frac{d\rho}{dt} = 0, \tag{1}$$

that is the phase-space density is conserved along the trajectories of the system.

We can express this in terms of partial derivatives

$$\frac{d\rho}{dt} = \frac{\partial \rho}{\partial t} + \frac{\partial \rho}{\partial q_i}\dot{q}_i + \frac{\partial \rho}{\partial p_i}\dot{p}_i = \frac{\partial \rho}{\partial t} + \frac{\partial \rho}{\partial q_i}\frac{\partial H}{\partial p_i} - \frac{\partial \rho}{\partial p_i}\frac{\partial H}{\partial q_i} = 0.$$

Hence we derive Liouville's Equation

$$\frac{d\rho}{dt} = \frac{\partial \rho}{\partial t} + \frac{\partial \rho}{\partial q_i}\frac{\partial H}{\partial p_i} - \frac{\partial \rho}{\partial p_i}\frac{\partial H}{\partial q_i} = 0.$$

This is an immediate consequence of Liouville's Theorem and Hamilton's Equations of motion.

5.3 Poisson Bracket

In last lecture we have derived Liouville's Equation

$$\frac{d\rho}{dt} = \frac{\partial \rho}{\partial t} + \frac{\partial \rho}{\partial q_i}\frac{\partial H}{\partial p_i} - \frac{\partial \rho}{\partial p_i}\frac{\partial H}{\partial q_i} = 0,$$

which follows Liouville's Theorem and Hamilton's Equations of motion. The structure of Liouville's Equation has a wider application.

For two functions on phase space, $f(q, p, t)$ and $g(q, p, t)$ the Poisson bracket is defined as

$$\{f, g\} = \frac{\partial f}{\partial q_i}\frac{\partial g}{\partial p_i} - \frac{\partial f}{\partial p_i}\frac{\partial g}{\partial q_i} \tag{1}$$

Properties of Poisson brackets:

(1) Anti-commutativity: $\{f, g\} = -\{g, f\}$.

(2) Linearity: $\{\alpha f + \beta g, h\} = \alpha\{f, h\} + \beta\{g, h\}$, $\forall\ \alpha, \beta \in \mathbb{R}$.

(3) Leibniz rule (follows from the chain rule): $\{fg, h\} = f\{g, h\} + \{f, h\}g$.

(4) Jacobi identity: $\{f, \{g, h\}\} + \{g, \{h, f\}\} + \{h, \{f, g\}\} = 0$.

(5) $\forall\ f(q, p, t)$

$$\frac{df}{dt} = \{f, H\} + \frac{\partial f}{\partial t}. \tag{2}$$

The latter expression is very useful. It can be interpreted as a generalization of Liouville's Theorem and is proved in exactly the same way.

Conserved quantities: An important consequence of (2) is that a function $g(q, p)$ on phase-space, which does not depend on time explicitly (i.e. $\frac{\partial g}{\partial t} = 0$) and satisfies $\{g, H\} = 0$, is a constant of motion.

It also follows from Jacobi identity that if g and h are constants of motion, then $\{g, h\}$ is also a constant of motion.

We discuss two examples:

(1) Angular Momentum $\boldsymbol{L} = \boldsymbol{r} \times \boldsymbol{p}$: in the example sheet 4 you will be asked to calculate several Poisson brackets for the AM. In particular, you can show that

$$\{L_1, L_2\} = L_3, \tag{3}$$

thus if two of its components are conserved, so is the third. In other words, AM is completely determined by any two of its components.

(2) (Laplace-)Runge-Lenz vector:
Consider motion of a particle of mass m. Let us define Laplace-Runge-Lenz vector

$$\boldsymbol{A} = \frac{\boldsymbol{p} \times \boldsymbol{L}}{m} - \hat{\boldsymbol{r}}, \tag{4}$$

where $\boldsymbol{p}$, $\boldsymbol{L}$ and $\hat{\boldsymbol{r}}$ are linear and angular momenta, and (normalized) position vector respectively. From definition of $\boldsymbol{L}$ it follows that $\boldsymbol{A} \cdot \boldsymbol{L} = 0$. In Example Sheet 4 you will be asked to show that $\{L_a, A_b\} = \epsilon_{abc} A_c$.

If the particle moves in a central force-field $\boldsymbol{F} = -kr^{-2}\hat{\boldsymbol{r}}$ (without loss of generality, let us assume that $k = 1$), then its Hamiltonian is

$$H = \frac{\boldsymbol{p}^2}{2m} - \frac{1}{r}. \tag{5}$$

In this case $\boldsymbol{A}$ is conserved (you will be asked to prove this statement by proving that $\{\boldsymbol{A}, H\} = 0$).

Conservation of $\boldsymbol{L}$ follows from the symmetry of the force field. Thus, $\boldsymbol{L}$, $\boldsymbol{A}$ and H form a closed algebra under the Poisson bracket.

Runge-Lenz vector has clear geometric interpretation. It is easy to show that the trajectory of the particle lies in the plane perpendicular to $\boldsymbol{L}$ (just calculate scalar product of $\boldsymbol{L}$ with $\boldsymbol{r}$ and $\dot{\boldsymbol{r}}$ - you must have done it in 1A Dynamics). Constant vector $\boldsymbol{A}$ also lies in the same plane. Let us calculate scalar product of $\boldsymbol{A}$ with $\boldsymbol{r}$. On the one hand,

$$\boldsymbol{A} \cdot \boldsymbol{r} = Ar\cos\theta, \tag{6}$$

where θ is the angle between the two vectors. On the other hand,

$$\boldsymbol{A} \cdot \boldsymbol{r} = \frac{(\boldsymbol{p} \times \boldsymbol{L}) \cdot \boldsymbol{r}}{m} - r = \frac{\boldsymbol{L}^2}{m} - r. \tag{7}$$

Hence we obtain the (familiar from 1A Dynamics) orbit equation

$$r = \frac{\boldsymbol{L}^2/m}{1 + A\cos\theta}, \tag{8}$$

where $A = e$ is the eccentricity of the orbit. Thus, $\boldsymbol{A}$ is directed along the axis of symmetry of the orbit with its magnitude being the eccentricity.

5.4 Canonical Transformations

In Hamiltonian Formalism we can treat generalized coordinates and momenta (almost) equally. This allows for a wider class of transformations, comparing with Lagrangian formalism. We can "mix" coordinates and momenta, so to speak:

$$\begin{cases} Q_i = Q_i(q,p), \\ P_i = P_i(q,p), \end{cases} \tag{1}$$

where Q_i and P_i, $i = 1, ..., n$, are $2n$ new independent variables. Of course, not any transformation will be good for us. We require that this transformation preserves canonical form of equations of motion, Hamilton's Equations, that is. Such transformations are called *canonical*. While Hamiltonian itself is not preserved necessarily, i.e. the new Hamiltonian $H'(Q,P)$ might not equal to $H(q,p)$, the equations of motion take the same form

$$\begin{cases} \dot{Q}_i = \dfrac{\partial H'}{\partial P_i}, \\ \dot{P}_i = -\dfrac{\partial H'}{\partial Q_i}. \end{cases} \tag{2}$$

How do we construct such transformations? We derive the formulae for canonical transformation $(q,p) \to (Q,P)$ using what is known as *generating function* $F(q,Q,t)$. It goes as follows.

Let us write the expression for the action integral in terms of q and p

$$S = \int_{t_1}^{t_2} (p_i\dot{q}_i - H(q,p))dt = \int_{t_1}^{t_2} (p_i dq_i - H dt), \tag{3}$$

where q_i and p_i are varied independently when we consider a variation $\delta S = 0$.
For Q_i and P_i to satisfy Hamilton's equations we require

$$S' = \int_{t_1}^{t_2} (P_i\dot{Q}_i - H'(Q,P))dt = \int_{t_1}^{t_2} (P_i dQ_i - H' dt), \tag{4}$$

where Q_i and P_i are varied independently when we consider a variation $\delta S' = 0$. For $\delta S = \delta S' = 0$ the intergrands in (3) and (4) must differ only by a full differential of an arbitrary function $F(q,Q,t)$[1] (a generating function). Hence,

$$dF = p_i dq_i - P_i dQ_i + (H' - H)dt, \tag{5}$$

and therefore

$$\begin{cases} p_i = \dfrac{\partial F}{\partial q_i}, \\ P_i = -\dfrac{\partial F}{\partial Q_i}, \\ H' = H + \dfrac{\partial F}{\partial t}. \end{cases} \tag{6}$$

Thus, F determines the relation between (q,p), (Q,P) and (H,H'). If F does not depend on time explicitly then new Hamiltonian H can be obtained by substituting $q(Q,P)$ and $p(Q,P)$ into H.

[1] There is not dependance on p and P because we do not neccessarily keep them fixed at t_1 and t_2 (see section 5.1)

(An alternative way to introduce canonical transformations is via Jacobian of the transformation. You will explore this route in the example sheet.)

We discuss the the following theorem.

Theorem 5.1 *The Poisson Bracket is invariant under Canonical Transformations, i.e. if the transformation* $(q,p) \to (Q,P)$ *is canonical, then for two function on phase-space,* $f(q,p)$ *and* $g(q,p)$*, the following relation holds*

$$\{f,g\}_{q,p} = \{f,g\}_{Q,P}. \tag{7}$$

We prove the sufficient condition in the lecture and leave the necessary condition for the example sheet.

Example: free particle
In order to appreciate the power of CT lets discuss a simple example of a free particle again. The Hamiltonian is $H = \boldsymbol{p}^2/2m$, where $\boldsymbol{p} = m\dot{\boldsymbol{r}}$. The Hamilton's equations take trivial form

$$\begin{cases} \dot{\boldsymbol{r}} = \dfrac{\partial H}{\partial \boldsymbol{p}} = \boldsymbol{p}/m, \\ \dot{\boldsymbol{p}} = -\dfrac{\partial H}{\partial \boldsymbol{r}} = 0. \end{cases} \tag{8}$$

Try the following generating function to find a new set of variables, $\boldsymbol{Q}$ and $\boldsymbol{P}$: $F(\boldsymbol{r},\boldsymbol{Q}) = \boldsymbol{r}\cdot\boldsymbol{Q}$. This yields

$$\begin{cases} \boldsymbol{p} = \dfrac{\partial F}{\partial \boldsymbol{r}} = \boldsymbol{Q}, \\ \boldsymbol{P} = -\dfrac{\partial H}{\partial \boldsymbol{Q}} = -\boldsymbol{r}, \\ H' = \dfrac{\boldsymbol{Q}^2}{2m}. \end{cases} \tag{9}$$

Hence, in this example the roles of spacial coordinate and momentum have been swapped! Thus the more general class of transformation allowed in Hamiltonian Formalism effectively removes the boundary between q and p. From now on we will call them simply *canonical conjugate variables.*