Lecture 5

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1 The Hamilton equations of motion

1.1 Legendre transformation and the Hamilton equations of motion

First-order equations of motion. In the Lagrangian formulation, a system with n degrees of freedom possesses n equations of motion of the form

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}}\right) - \frac{\partial L}{\partial q} = 0 \tag{1}$$

As the equations are of second order, the motion of the system for all moments of time is determined when $2n$ initial values at $t = t_1$:

$$\text{initial values} = \begin{cases} q_i(t_1), & i = 1, \dots n \\ \dot{q}_i(t_1), & i = 1, \dots n \end{cases} \tag{2}$$

Lagrange equations of motion describe a *trajectory* in the n-dimensional *configuration space* $(q_1(t), \dots, q_n(t))$.

Instead of the 2nd order in time evolution of functions $q_i(t)$ we can rewrite the system as $2n$ first order differential equation on the variables $q_i(t); \dot{q}_i(t)$:

$$\begin{cases} y_i & \equiv & \dot{q}_i \\ \dfrac{d}{dt}\dfrac{\partial L(q,y)}{\partial y_i} & = & \dfrac{\partial L}{\partial q_i}(q,y) \end{cases} \tag{3}$$

The second equation implicitly contains $\dot{y}_i$ in its left-hand-side, but *it is not resolved explicitly for it*. We would like to bring these equations to the form:

$$\frac{d}{dt}\vec{X} = \mathcal{F}[\vec{X}(t), t] \tag{4}$$

where $\vec{X} = (q_1, \dots . . q_n, \dot{q}_1, \dots \dot{q}_n)$ is a $2n$-dimensional vector.

In order to do that, we introduce *generalised momenta* p_i via

$$p_i(t) \equiv \frac{\partial L(q, \dot{q})}{\partial \dot{q}_i} \tag{5}$$

such that the second Lagrange equation (3) simplifies to become

$$\frac{dp_i}{dt} = \frac{\partial L(q,\dot{q})}{\partial q_i} \tag{6}$$

This, however, does not realize our goal, because equations (6) contain *three variables:* q, p *and* $\dot{q}$. To solve this issue, let us express generalised velocities $\dot{q}_i$ as functions of q_i and p_i in Eqn (5):

$$\dot{q}_i = \dot{Q}_i(q,p) \Longrightarrow p_i = \left.\frac{\partial L(q,\dot{q},t)}{\partial \dot{q}_i}\right|_{\dot{q}_i=\dot{Q}_i(q,p)} \tag{7}$$

we will obtain a system of $2n$ first order equations for the independent variables q_i and p_i

$$\boxed{\begin{cases} \dot{q}_i = \dot{Q}_i(q,p) \\ \dot{p}_i = P_i(q,p) \equiv \left.\dfrac{\partial L(q,\dot{q}),t)}{\partial q_i}\right|_{\dot{q}_i=\dot{Q}_i(q,p)} \end{cases}} \tag{8}$$

1.2 Hamiltonian

We see, that to find needed equations can be not a trivial problem, so we need to have a general procedure to solve it. We need to solve mathematical problem of the transition from variables in our mechanical functions from $(q,\dot{q})$ to (q,p), where p's are related to q and $\dot{q}$ by eqs (5): $p = \frac{\partial L}{\partial \dot{q}}$. We will introduce a new function $H(p,q) = p\dot{q} - L(q,\dot{q})\Big|_{\dot{q}=Q(q,p)}$ such that

$$\frac{\partial H}{\partial q} = -\frac{\partial L}{\partial q} = -\dot{p} \tag{9}$$

and it allows to resolve $\dot{q}$ as a function of q, p via

$$\dot{q} = \frac{\partial H}{\partial p} \tag{10}$$

To see this, we begin by writing the differential of the Lagrangian, $L(q,\dot{q})$, as (using the notation $y \equiv \dot{q}$ to keep formulas simple):

$$dL(q,y) = \frac{\partial L}{\partial q}dq + \frac{\partial L}{\partial y}dy \tag{11}$$

which we can write using (6) as

$$dL = \dot{p}dq + pdy \tag{12}$$

using obvious identity

$$d(py) = ydp + pdy \tag{13}$$

we subtract $d(py)$ from both sides of Eq. (12) and get rid of pdy term in the right hand side of Eq. (12).

As a result we define a *new function* called **Hamiltonian** $H(q,p)$

$$\boxed{H(q,p) \equiv p\dot{q} - L(q,\dot{q})\Big|_{\dot{q}=Q(q,p)}} \tag{14}$$

such that

$$dH(q,p) = \dot{q}dp - \dot{p}dq \tag{15}$$

On the other hand of course as any function of q, p

$$dH = \frac{\partial H}{\partial p}dp + \frac{\partial H}{\partial q}dq \tag{16}$$

Comparing (15) and (16) we find

$$\left.\begin{aligned} \dot{q} &= \frac{\partial H}{\partial p} \\ \dot{p} &= -\frac{\partial H}{\partial q} \end{aligned}\right\} \qquad \textbf{Hamilton equations} \tag{17}$$

Eqs. (14), (15), (16) are trivially generalized to the case when there n coordinates q_i:

$$H(q_i, p_i) = \sum_i p_i \dot{q}_i - L(q_i, \dot{q}_i) \tag{18}$$

and

$$\begin{aligned} \dot{q}_i &= \frac{\partial H}{\partial p_i} \\ \dot{p}_i &= -\frac{\partial H}{\partial q_i} \end{aligned} \tag{19}$$

Equations (19) are known as the *canonical equations of Hamilton*; they constitute the desired set of $2n$ first-order equations of motion replacing the n second-order Lagrange equations.

The first half of Hamilton's equations give the $\dot{q}_i$ as functions of (q, p, t). They form therefore the inverse of the constitutive equations (5), which define the momenta p_i as functions of $(q, \dot{q}, t)$. It may therefore be said that they provide no new information. In terms of solving mechanical problems by means of the canonical equations, the statement is correct. But within the framework of the Hamiltonian picture, where $H(q, p, t)$ is some given function obtained no matter how, the two halves of the set of Hamiltonian equations are equally independent and meaningful. The first half says how $\dot{q}$ depends on q, p, and t; the second says the same thing for $\dot{p}$.

Constructing a Hamiltonian. Formally, the Hamiltonian for each problem must be constructed starting from the Lagrangian as follows:

1. With a chosen set of generalized coordinates, q, the Lagrangian $L(q, \dot{q}, t) = T - V$ is constructed.

2. The conjugate momenta are defined as functions of q, $\dot{q}$, and t via eqs. (5).

3. Equation (14) is used to form the Hamiltonian. At this stage we have some mixed function of q, $\dot{q}$, p, and t.

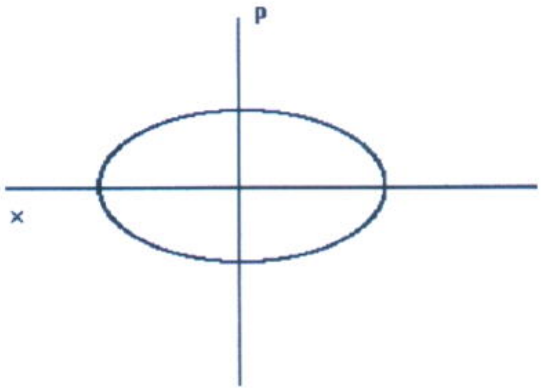

Figure 1: Trajectory in the *phase space* $(q(t), p(t))$ governed by the Hamiltonian equation (17).

4. Equations (5) are then inverted to obtain $\dot{q}_i$'s as functions of (q, p, t). Possible difficulties in the inversion will be discussed below.

5. The results of the previous step are then applied to eliminate $\dot{q}$ from H so as to express it solely as a function of (q, p, t).

Of course, the Hamiltonian H is just the energy function, $E(q, \dot{q})$ defined in previous lecture. But they are functions of different variables: like the Lagrangian, E is a function of q, $\dot{q}$ (and possibly t), while H must always be expressed as a function of q, p (and possibly t). It is to emphasize this difference in functional behavior that different symbols have been given to the quantities even though they have the same numerical values.

Therefore, the following procedure can be used: build the *energy* of the system E as $E = T + U$. Then express $\dot{q}_i$'s in $E(q, \dot{q}, t)$ via p_i's using equations (5). The resulting $E(q, \dot{Q}(q, p) = H(q, p)$ is the desired Hamiltonian.

1.3 Hamiltonian variation principle

The Hamiltonian equations (17) can be obtained from a variational principle, similar to their Lagrangian counterparts.

Recall, that the Lagrange equations could be obtained as equations for the extremum of the functional $S_L[q(t), \dot{q}(t)]$:

$$S_L = \int dt\, L(q, \dot{q}) \tag{20}$$

Let us re-express the Lagrangian as $L = p\dot{q} - H(p, q)$ and consider the variation of the action

$$S_H = \int dt \underbrace{\Big[p\dot{q} - H(q, p)\Big]}_{\equiv F(p,\dot{p},q,\dot{q})} \tag{21}$$

This time the variation takes place in the *phase space* (i.e. one considers a trajectory $\big(q(t), p(t)\big)$ and its variation $\big(q(t) + \delta q(t), p(t) + \delta p(t)\big)$. The variational principle gives

then the analog of Lagrange equations in the phase space:

$$\frac{d}{dt}\left(\frac{\partial F}{\partial \dot{p}}\right) - \frac{\partial F}{\partial p} = 0 \tag{22}$$

$$\frac{d}{dt}\left(\frac{\partial F}{\partial \dot{q}}\right) - \frac{\partial F}{\partial q} = 0 \tag{23}$$

Notice, that the function F, introduced in (21) depends on $\dot{q}$ only via the term $p\dot{q}$. Therefore, we can rewrite (23) as

$$\dot{p} = -\frac{\partial H}{\partial q} \tag{24}$$

On the other hand, F does *not* depend on $\dot{p}$ and depends on q only via the term $H(p,q)$. This gives us (from (22))

$$\frac{\partial F}{\partial p} = \dot{q} - \frac{\partial H}{\partial p} = 0 \tag{25}$$

1.4 Examples of Hamiltonians

1.4.1 Particle in centrally symmetric potential

First consider the spatial motion of a particle in a central force field, using spherical polar coordinates (r, θ, φ) for the generalized coordinates. The potential energy is some function $V(r)$ and the kinetic energy is

$$T = \frac{mv^2}{2} = \frac{m}{2}(\dot{r}^2 + r^2\dot{\varphi}^2\sin^2\theta + r^2\dot{\theta}^2) \tag{26}$$

We have

$$p_r = \frac{\partial L}{\partial \dot{r}} = m\dot{r}; \quad p_\theta = \frac{\partial L}{\partial \dot{\theta}} = mr^2\dot{\theta}; \quad p_\phi = \frac{\partial L}{\partial \dot{\phi}} = mr^2\sin^2\theta\dot{\phi} \tag{27}$$

Clearly the Hamiltonian has the form of $T + V$, so

$$H(r, \theta, p_r, p_\theta, p_\varphi) = \frac{1}{2m}\left(p_r^2 + \frac{p_\theta^2}{r^2} + \frac{p_\varphi^2}{r^2\sin^2\theta}\right) + V(r) \tag{28}$$

Note that in Cartesian coordinates we have:

$$T = \frac{mv^2}{2} = \sum_i \frac{m\dot{x}_i^2}{2} \tag{29}$$

so that the Hamiltonian is now

$$H = \sum_i \frac{\dot{p}_i^2}{2m} + V(r) = \frac{\vec{p}^{\,2}}{2m} + V(r) \tag{30}$$

We can of course take the components of $\vec{p}$ relative to any coordinate system we desire, curvilinear spherical coordinates, for example. But it is important not to confuse, say, p_θ with the θ component of $\vec{p}$. The former is the canonical momentum conjugate to the coordinate θ; the latter is the θ component of the momentum vector conjugate to the Cartesian coordinates. Dimensionally, it is clear they are quite separate quantities; p_θ is an angular momentum, $(\vec{p})_\theta$ is linear momentum.

1.4.2 Hamiltonian of a particle in electromagnetic field.

For a second example, let us consider a single (nonrelativistic) particle of mass m and charge q in the electromagnetic field. The Lagrangian is given by Eq. (31)

$$L = \frac{m\vec{v}^2}{2} - q\varphi + q\vec{A}\cdot\vec{v} \tag{31}$$

The canonical momenta $\vec{p}$ are given by

$$\vec{p} = \frac{\partial L}{\partial \vec{v}} = m\vec{v} + q\vec{A} \tag{32}$$

and the Hamiltonian is:

$$H = \vec{p}\cdot\vec{v} - L(\vec{v}) \tag{33}$$

The term linear in $\vec{v}$ cancels out under the transformation (33) and as a result we get:

$$H = \frac{(\vec{p} - q\vec{A})^2}{2m} + q\varphi \tag{34}$$

which is the total energy of the particle in the electromagnetic field. Using the Hamiltonian (34) it is easy to obtain the equations of motion (35) and (36) (*check this*):

$$\frac{d\vec{x}}{dt} = \frac{\vec{p} - q\vec{A}(x)}{m} \tag{35}$$

$$\frac{d\vec{p}}{dt} = -q\frac{\partial\varphi}{\partial\vec{x}} + \frac{q}{m}\frac{\partial\vec{A}}{\partial\vec{x}}\cdot(\vec{p} - q\vec{A}) \tag{36}$$

1.4.3 Relativistic particle. Lagrangian (reminder) and Hamiltonian

We saw in the previous lecture that the Lagrangian of a relativistic particle is given by the

$$L = -mc^2\sqrt{1-\beta^2}, \quad \text{where} \quad \beta^2 = \frac{\vec{v}^{\,2}}{c^2} \tag{37}$$

If the relativistic particle moves in the external potential $V(\vec{r})$, the Lagrangian becomes

$$L = -mc^2\sqrt{1-\beta^2} - V(\vec{r}) \tag{38}$$

Let us construct the generalized momentum $\vec{p}$:

$$\vec{p} = \frac{\partial L}{\partial \vec{v}} = \frac{m\vec{v}}{\sqrt{1-\beta^2}} \tag{39}$$

– the expression that is known as momentum of a relativistic particle. It approaches $m\vec{v}$ as $\beta \to 0$ (non-relativistic limit). The 3-dimensional part of the equations of motion has the form:

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \vec{v}}\right) - \frac{\partial L}{\partial \vec{r}} = \frac{d\vec{p}}{dt} + \nabla V(\vec{r}) = 0 \tag{40}$$

– we recovered the second Newton's law for potential force $\vec{F} = -\nabla V$ that is known to remain true also in relativistic case.

We can construct energy for the Lagrangian (38), given by

$$\mathcal{E} = \vec{v}\frac{\partial L}{\partial \vec{v}} - L = \frac{m\vec{v}^2}{\sqrt{1-\beta^2}} + mc^2\sqrt{1-\beta^2} + V(\vec{r}) = \frac{mc^2}{\sqrt{1-\beta^2}} + V(\vec{r}) \tag{41}$$

(where we see the kinetic energy of relativistic particle plus potential energy). Indeed,

$$\frac{mc^2}{\sqrt{1-\beta^2}} = \begin{cases} mc^2, & \text{if} \quad \beta = 0 \leftarrow \quad \text{rest energy} \\ mc^2 + \dfrac{mv^2}{2}, & \text{if} \quad 0 < \beta \ll 1 \leftarrow \quad \text{non-relativistic limit} \\ \to \infty, & \text{if} \quad \beta \to 1 \leftarrow \quad \text{ultra-relativistic limit} \end{cases} \tag{42}$$

Let us also consider the case when the relativistic particle moves in the electromagnetic field. We saw that this amounts to adding the potential $U(\vec{r},\vec{v}) = q\phi - q\vec{A}\cdot\vec{v}$. We can build the Lagrange equations in this case, an analog of eq. (40):

$$\frac{d\vec{P}}{dt} = q\vec{E} + q\vec{v}\times\vec{B} \tag{43}$$

– similar to Eq. (40) with the only difference that the *generalized momentum* $\vec{P}$ is

$$\vec{P} \equiv \frac{\partial L}{\partial \vec{v}} = \frac{m\vec{v}}{\sqrt{1-\beta^2}} + q\vec{A} \tag{44}$$

1.4.4 Relativistic particle in the constant electric field.

Consider the situation when the particle is accelerating under constant force – electron in an electric field. The Lagrangian has the form

$$L = -mc^2\sqrt{1-\beta^2} + eEx \tag{45}$$

(charge of electron $q = -e$, $e > 0$). The Lagrange equation:

$$\frac{d}{dt}\left(\frac{\partial L}{\partial v_x}\right) - \frac{\partial L}{\partial x} = \frac{d}{dt}\left(\frac{mc\beta}{\sqrt{1-\beta^2}}\right) - eE = 0 \tag{46}$$

Therefore

$$\frac{d}{dt}\left(\frac{\beta(t)}{\sqrt{1-\beta(t)^2}}\right) = \frac{eE}{mc} \tag{47}$$

The velocity (recall that $\beta(t) = \frac{v_x}{c}$) is given by

$$\beta = \frac{\frac{eE}{mc}t}{\sqrt{1+\left(\frac{eE}{mc}t\right)^2}} \tag{48}$$

Notice, that the solution (48) automatically ensures $\beta < 1$ and that $\beta \to 1$ as $t \to \infty$ – being left for infinitely long time the electron will accelerate, approaching the speed of light (see Fig. 2).

Integrating Eq. (48) over time, we find

$$x(t) = \frac{mc^2}{eE}\left(\sqrt{1+\left(\frac{eE}{mc}t\right)^2} - 1\right) \tag{49}$$

In the low-velocity limit:

$$v_x(t) = \frac{eE}{m}t, \quad x(t) = \frac{eE}{2m}t^2 \qquad \beta \ll 1 \tag{50}$$

As time goes to infinity, solution (49) approaches $x = ct$ (see Fig. 2).

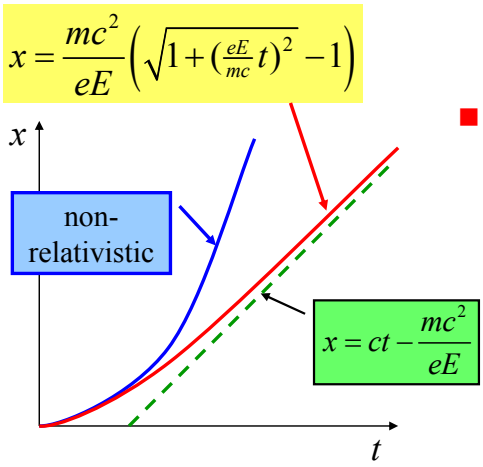

Figure 2: Trajectory $x(t)$ of an electron, accelerated by a constant electric field.

Same system, Hamiltonian equations. Let us now repeat the same exercise in the Hamiltonian Language. Starting with Eq. (45) we write:

$$p_x = \frac{\partial L}{\partial v_x} = \frac{mv_x}{\sqrt{1-\beta^2}}, \qquad \text{where} \quad \beta = \frac{v_x}{c} \tag{51}$$

We can invert the expression (51) to express β via p_x:

$$\beta = \frac{p_x}{\sqrt{m^2c^2 + p_x^2}} \tag{52}$$

The Hamiltonian is *energy* in this case, i.e.

$$H(x, p_x) = \sqrt{p_x^2c^2 + m^2c^4} - exE \tag{53}$$

Indeed

$$p_xv_x - L(x, v_x) = \frac{mv_x^2}{\sqrt{1-\beta^2}} + mc^2\sqrt{1-\beta^2} - eEx = \frac{mc^2}{\sqrt{1-\beta^2}} - eEx \tag{54}$$

Using $\beta(p_x)$ from (52) we arrive to (53). The Hamiltonian equations have the form:

$$\dot{p}_x = -\frac{\partial H}{\partial x} = eE \tag{55}$$

$$\dot{x} = \frac{\partial H}{\partial p_x} = \frac{p_x}{\sqrt{p_x^2 + m^2c^2}} \tag{56}$$

Integrating Eq. (55) we get

$$p_x = eEt \tag{57}$$

(as in the previous example, we choose $p_x(0) = 0$ to simplify the expressions). Thus, substituting (57) in (56) we arrive again to the Eq. (48) and therefore to the solution (49).

1.5 Liouville's theorem. Canonical transformations

While the exact motion of any system is completely determined in classical mechanics by the initial conditions, it is often impracticable to calculate an exact solution for complex systems. It would be obviously hopeless, for example, to calculate completely the motion of some 10^{23} molecules in a volume of gas. In addition, the initial conditions are often only incompletely known. We may be able to state that at time to a given mass of gas has a certain energy, but we cannot determine the initial coordinates and velocities of each molecule. Statistical mechanics therefore makes no attempt to obtain a complete solution for systems containing many particles. Its aim, instead, is to make predictions about certain average properties by examining the motion of a large number of identical systems. The values of the desired quantities are then computed by forming averages over all the systems in the ensemble. All the members of the ensemble are as like the actual systems as our imperfect knowledge permits, but they may have any of the initial conditions that are consistent with this incomplete information. Since each system is represented by a single point in phase space, the ensemble of systems corresponds to a swarm of points in phase space. **Liouville's theorem** states that *the density of systems in the neighborhood of some given system in phase space remains constant in time* (see 9.9 of [3]).

The density can vary with time through two separate mechanisms. Since it is the density in the neighborhood of a given system point,there will be an implicit dependence as the coordinates of the system (q, p) vary with time, and the system point wanders through phase space. There may also bean explicit dependence upon time. The density may still vary with time even when evaluated at a fixed point in phase space.

The ensemble of system points moving through phase space behaves much like a fluid in a multidimensional space, and there are numerous similarities between our discussion of the ensemble and the well-known notions of fluid dynamics.

Consider an infinitesimal volume $d\Omega$ in phase space surrounding a given system point, with the boundary of the volume formed by some surface of neighboring system points at the time $t = 0$. Note that the surface of the volume is one-dimension less than the volume. In the course of time, the system points defining the volume move about in phase space, and the volume contained by them will take on different shapes as time progresses. The dashed curve in fig. 3 indicates the evolution of the infinitesimal volume with time. It is clear that the number of systems dN within the volume remains constant, for a system initially inside can never get out. If some system point were to cross the border, it would occupy at some time the same position in phase space as one of the system points defining the boundary surface. Since the subsequent motion of a system is uniquely determined by its location in phase space at a particular time, the two systems would travel together from there on. Hence, the system can never leave the volume. By the same token, a system initially outside can never enter the volume.

From another side let's look how the volume dV changes in the process of evolution of a system. Namely, we start with the region $d\Omega$ at time t_1 and consider the evolution from t_1 to t_2 as a change of variables of the phase space region $d\Omega$.

$$\begin{aligned} q_i' &= q_i(t_2) \\ p_i' &= p_i(t_2) \end{aligned} \tag{58}$$

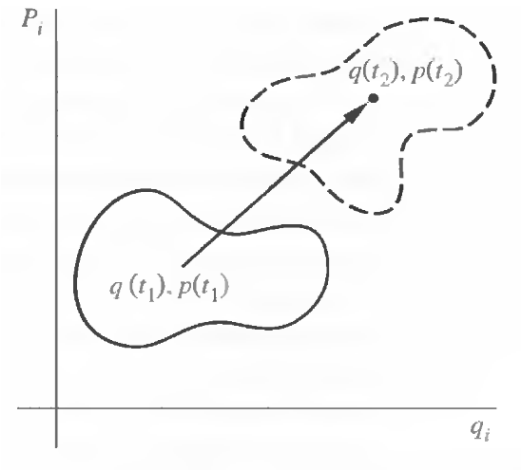

Figure 3: Motion of a volume in two-dimensional phase space.

The volume of Ω_{t_1} is given by

$$V_{t_1} = \int\limits_{\Omega_{t_1}} \prod_{i=1}^{n} dq_i dp_i \tag{59}$$

at time t_1 and

$$V'_{t_2} = \int\limits_{\Omega_{t_2}} \prod_{i=1}^{n} dq'_i dp'_i \tag{60}$$

at time t_2.

Under any change of variables (58) the volume transforms as

$$V'_{t_2} = \int\limits_{\Omega_{t_1}} J \prod_{i=1}^{n} dq_i dp_i \tag{61}$$

where

$$J = \frac{\partial(q'_1, \ldots, q'_n, p'_1, \ldots, p'_n)}{\partial(q_1, \ldots, q_n, p_1, \ldots, p_n)} \tag{62}$$

is Jacobian of the transition. Note, them integration phase volume $d\Omega'$ becomes to $d\Omega$ just because of $d\Omega'$ definition. Using Hamilton equations of motion (19) we have

$$q'_i = q_i + \delta q_i = q_i + \dot{q}_i \delta t = q_i + \frac{\partial H}{\partial p_i} \delta t \tag{63}$$

$$p'_i = p_i + \delta p_i = p_i + \dot{p}_i \delta t = p_i - \frac{\partial H}{\partial q_i} \delta t \tag{64}$$

Let's look at the simplest situation $n = 1$. Then we have:

$$J = \begin{vmatrix} \frac{\partial q'}{\partial q} & \frac{\partial q'}{\partial p} \\ \frac{\partial p'}{\partial q} & \frac{\partial p'}{\partial p} \end{vmatrix} = \begin{vmatrix} 1 + \frac{\partial^2 H}{\partial p \partial q}\delta t & \frac{\partial^2 H}{\partial p^2}\delta t \\ -\frac{\partial^2 H}{\partial q^2}\delta t & 1 - \frac{\partial^2 H}{\partial p \partial q}\delta t \end{vmatrix} =$$

$$= 1 - \left(\frac{\partial^2 H}{\partial p \partial q}\right)^2 \delta t^2 + \frac{\partial^2 H}{\partial p^2}\frac{\partial^2 H}{\partial q^2}\delta t^2 = 1 + O(\delta t^2) \quad (65)$$

Expression for J doesn't contain linear in δt term. This means that we can consider $J = 1$ for infinitesimal time interval. Therefore we straightly have

$$dV' = \int\limits_{\Omega} J \prod_{i=1}^{n} dq_i dp_i = dV \quad (66)$$

for every infinitesimal time shift, so this is true for finite time shift. We obtain this result for case $n = 1$, but it's true for any $n > 1$, the proof is very similar.

Thus, both the number of systems in the infinitesimal region, dN, and the volume, dV, are constants, and consequently the density

$$D = \frac{dN}{dV} \quad (67)$$

must also be constant in time, that is,

$$\frac{dD}{dt} = 0 \quad (68)$$

which proves Liouville's theorem.

When the ensemble of systems is in statistical equilibrium, the number of systems in a given state must be constant in time, which is to say that the density of system points at a given spot in phase space does not change with time. The variation of D with time at a fixed point corresponds to the partial derivative with respect to t, which therefore must vanish in statistical equilibrium.

We can ensure equilibrium therefore by choosing the density D to be a function of those constants of the motion of the system not involving time explicitly, for then the Poisson bracket with H must vanish. Thus, for conservative systems D can be any function of the energy, and the equilibrium condition is automatically satisfied.

The considerations have been presented here to illustrate the usefulness of the Hamilton formulation of classical mechanics. Further discussion of these points would carry us far outside our field.

1.6 Poisson brackets

To see the power of Hamilton formulation of mechanics we need to add a new conception, called Poisson brackets (see paragraph 42 of [2]).

Let $f(p,q)$ be some function of coordinates, momenta. Let its dependence on time be via $q(t)$ and $p(t)$, i.e. $f(t) = f\big(q(t), p(t)\big)$. Its total time derivative is

$$\frac{df}{dt} = \sum_i \left(\frac{\partial f}{\partial q_i}\dot{q}_i + \frac{\partial f}{\partial p_i}\dot{p}_i \right) = \sum_i \left(\frac{\partial f}{\partial q_i}\frac{\partial H}{\partial p_i} - \frac{\partial f}{\partial p_i}\frac{\partial H}{\partial q_i} \right) \tag{69}$$

Substitution of the values of $\dot{q}$ and $\dot{p}$ given by Hamilton's equations (19) leads to the expression

$$\frac{df}{dt} = [f, H] \tag{70}$$

where we have introduced a notation:

$$[f, H] \equiv \sum_i \left(\frac{\partial f}{\partial q_i}\frac{\partial H}{\partial p_i} - \frac{\partial f}{\partial p_i}\frac{\partial H}{\partial q_i} \right) \tag{71}$$

This expression is called the **Poisson bracket** of the quantities H and f.[1]

For any two quantities f and g, the Poisson bracket is defined analogously to (71):

$$[f, g] = \sum_i \left(\frac{\partial f}{\partial q_i}\frac{\partial g}{\partial p_i} - \frac{\partial f}{\partial p_i}\frac{\partial g}{\partial q_i} \right) \tag{72}$$

Poisson bracket with q and p: If one of the functions f and g is one of the momenta or coordinates, the Poisson bracket reduces to a partial derivative:

$$[f, q_k] = -\frac{\partial f}{\partial p_k} \tag{73}$$

$$[f, p_k] = \frac{\partial f}{\partial q_k} \tag{74}$$

so we have:

$$[q_i, q_k] = 0, \quad [p_i, p_k] = 0, \quad [q_i, p_k] = \delta_{ik} \tag{75}$$

This allows to write the Hamiltonian equations in the following form:

$$\boxed{\begin{aligned} \frac{\partial q_i}{\partial t} &= [q_i, H] \\ \frac{\partial p_i}{\partial t} &= [p_i, H] \end{aligned}} \tag{76}$$

or, introducing a vector in $2n$-dimensional phase space $\vec{\eta} = (q_1, \ldots, q_n, p_1, \ldots, p_n)$:

$$\frac{d\vec{\eta}}{dt} = [\vec{\eta}, H] \tag{77}$$

[1] So far we have considered the case when the function f depends on time only via $q(t)$ and $p(t)$. In which case the Eq. (70) holds. In a more general case f can also explicitly depend on time $f = f(t, q(t), p(t))$. In this case Eq. (70) becomes:

$$\boxed{\frac{df}{dt} = \frac{\partial f}{\partial t} + [f, H]}$$

Those functions of the dynamical variables which remain constant during the motion of the system are called **integrals of the motion**. We see from (70) that the condition for the quantity f to be an integral of the motion ($df/dt = 0$) can be written[2]

$$[f, H] = 0 \tag{78}$$

The Poisson bracket has the following properties, which are easily derived from its definition.

1.6.1 Properties of the Poisson bracket

Antisymmetric. If the two functions are interchanged, the bracket changes sign:

$$[f, g] = -[g, f] \tag{79}$$

If one of the functions is a constant, the bracket is zero:

$$[f, c] = 0 \tag{80}$$

Linear operation:

$$[f_1 + f_2, g] = [f_1, g] + [f_2, g] \tag{81}$$

(82)

Leibnitz rule:

$$[f_1 f_2, g] = f_1[f_2, g] + f_2[f_1, g] \tag{83}$$

Taking the partial derivative of (72) with respect to time, we obtain

$$\frac{\partial}{\partial t}[f, g] = \left[\frac{\partial f}{\partial t}, g\right] + \left[f, \frac{\partial g}{\partial t}\right] \tag{84}$$

Jacobi's identity For any three functions of (q, p)

$$[[f, g], h] + [[g, h], f] + [[h, f], g] = 0 \tag{85}$$

1.6.2 Integrals of motion

An important property of the Poisson bracket is that

if f and g are two integrals of the motion, their Poisson bracket is likewise an integral of the motion:

[2] If the integral of the motion explicitly depends on time, then instead of Eq. (78) we should write

$$\frac{\partial f}{\partial t} + [f, H] = 0$$

$$[f, g] = \text{constant} \tag{86}$$

This is Poisson's theorem. The proof is very simple if f and g do not depend explicitly on the time. Putting $h = H$ in Jacobi's identity, we obtain

$$[[f, g], H] + [[g, H], f] + [[H, f], g] = 0 \tag{87}$$

Hence, if $[g, H] = 0$ and $[f, H] = 0$, then $[[f, g], H] = 0$, which is the required result.

If the integrals f and g of the motion are explicitly time-dependent, we put, from (70),

$$\frac{d}{dt}[f, g] = \frac{\partial}{\partial t}[f, g] + [[f, g], H] \tag{88}$$

Using formula (84) and expressing the bracket $[[f, g], H]$ in terms of two others by means of Jacobi's identity, we find

$$\begin{aligned} \frac{d}{dt}[f, g] &= \left[\frac{\partial f}{\partial t}, g\right] + \left[f, \frac{\partial g}{\partial t}\right] - [[g, H], f] - [[H, f], g] = \\ &= \left[\frac{\partial f}{\partial t} + [f, H], g\right] + \left[f, \frac{\partial g}{\partial t} + [g, H]\right] = \left[\frac{df}{dt}, g\right] + \left[f, \frac{dg}{dt}\right] = 0 \end{aligned} \tag{89}$$

which evidently proves Poisson's theorem.

Of course, Poisson's theorem does not always supply further integrals of the motion, since there are only $2n - 1$ of these (n being the number of degrees of freedom). In some cases the result is trivial, the Poisson bracket being a constant. In other cases the integral obtained is simply a function of the original integrals f and g. If neither of these two possibilities occurs, however, then the Poisson bracket is a further integral of the motion.

1.6.3 Examples of Poisson bracket usage

To illustrate the usage of Poisson bracket let's consider a system in which p_x and

$$M_z = xp_y - yp_x$$

components of momentum and angular momentum are conserved. Let us calculate

$$[p_x, M_z] = [p_x, (xp_y - yp_x)] \tag{90}$$

Using Eqs. (83), (81) and (75) we write

$$\begin{aligned} [p_x, M_z] &= [p_x, x]p_y - x\cancelto{0}{[p_x, p_y]} - \cancelto{0}{[p_x, y]}p_x + y\cancelto{0}{[p_x, p_x]} \\ &= -p_y \end{aligned} \tag{91}$$

(where in last line we used that $[x, p_x] = 1$).

So, we have found, using the Poisson's theorem, that *if p_x and M_z are conserved then p_y is conserved for any system.*[3]

[3] Of course, this result is easy to understand, as conservation of M_z implies axial symmetry with respect to z axis. Thus p_x and p_y should be interchangeable and if one is conserved, so should another.

1.6.4 Integrals of motions as generators of transformations

We can use any integral of motion (such as momentum $\vec{p}$ or the angular momentum $\vec{M}$) to generate transformations of q and p.

Translation. Consider the integral of motion p_x and its Poisson bracket with q. This gives

$$\begin{aligned} \frac{dx}{du} &= [x, p_x] = 1 \\ \frac{dy}{du} &= [y, p_x] = 0 \\ \frac{dz}{du} &= [z, p_x] = 0 \end{aligned} \tag{92}$$

The solution is therefore $x(u) = x_0 + u$. As one could guess, p_x generates translation along x axis!

Rotation. Let us look at the transformation of q and p generated by M_z:

$$\begin{aligned} \frac{dx}{d\phi} &= [x, M_z] = [x, (xp_y - yp_x)] = -y \\ \frac{dy}{d\phi} &= [y, M_z] = [y, (xp_y - yp_x)] = x \\ \frac{dz}{d\phi} &= [z, M_z] = [z, (xp_y - yp_x)] = 0 \end{aligned} \tag{93}$$

This can be re-written as

$$\frac{d}{d\phi}\begin{pmatrix} x(\phi) \\ y(\phi) \\ z(\phi) \end{pmatrix} = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} x(\phi) \\ y(\phi) \\ z(\phi) \end{pmatrix} \tag{94}$$

The matrix

$$\mathcal{M}_z = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \tag{95}$$

that appeared is the matrix of rotation around z-axis. We see that the angular momentum M_z generate rotations around the z-axis via the Poisson bracket.

Group of rotation. Indeed, let us start with considering a 2×2 matrix of rotation in the plane. By definition *rotation* is something that preserve the length of any Euclidean vector. Therefore, taking any matrix X and any vector $\vec{a} = (a_x, a_y)$ we should find that

$$(\vec{a}')^2 = (X \cdot \vec{a})^2, \quad \text{where} \quad \vec{a}\,' = X\vec{a} \tag{96}$$

Eq. (96) means that

$$X^T X = \mathbb{1} \tag{97}$$

Notice that $\det(X^T X) = (\det X)^2 = 1$.

Taking a generic matrix

$$X = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \tag{98}$$

we find 3 conditions (the 4th equations is identical to the second line)

$$\begin{cases} a^2 + c^2 = 1 \\ ab + cd = 0 \\ b^2 + d^2 = 1 \end{cases} \tag{99}$$

Let us assume $a \neq 0$, then we can write

$$c = \pm\sqrt{1 - a^2} \tag{100}$$

$$b = -\frac{cd}{a} \tag{101}$$

$$\left(\frac{cd}{a}\right)^2 + d^2 = 1 \tag{102}$$

Line (102) taking into account (99) leads to

$$a^2 = d^2 \tag{103}$$

Therefore $a = \pm d$ and as a result of (101) $b = \mp c$. In addition to that the determinant of the matrix X is given by

$$\det X = ad - bc = \pm(a^2 + c^2) = \pm 1 \tag{104}$$

where the upper sign corresponds to the choice $a = d$ and $b = -c$, while the lower sign is for the opposite case.

Let us concentrate on the case $\det X = 1$. In this case a, b, c, d can be parametrized via one *angle* ϕ as follows:

$$X(\phi) = \begin{pmatrix} \cos\phi & -\sin\phi \\ \sin\phi & \cos\phi \end{pmatrix} \tag{105}$$

This matrix takes any vector (a_x, a_y) and rotates it by angle ϕ:

$$\begin{pmatrix} a'_x \\ a'_y \end{pmatrix} = \begin{pmatrix} \cos\phi & -\sin\phi \\ \sin\phi & \cos\phi \end{pmatrix} \begin{pmatrix} a_x \\ a_y \end{pmatrix} \tag{106}$$

Consider an infinitesimal rotation, i.e $\phi \ll 1$. The matrix is then becomes close to the unity matrix:

$$X(\phi \ll 1) \approx \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + \phi \underbrace{\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}}_{\equiv \mathcal{X}} + \mathcal{O}(\phi^2) \tag{107}$$

Notice, that matrix $\mathcal{M}_z$ has the block-diagonal form with $\mathcal{X}$ in the upper left corner:

$$\mathcal{M}_z = \left(\begin{array}{c|c} \mathcal{X} & 0 \\ \hline 0 & 0 \end{array}\right) \tag{108}$$

The main property of the matrix $\mathcal{X}$ is

$$\mathcal{X}^2 = -\mathbb{1} \tag{109}$$

Notice, that we could recover the matrix $X(\phi)$ for arbitrary ϕ by defining a *matrix exponent* of the matrix $\mathcal{X}$:

$$\begin{aligned} X(\phi) = e^{\phi\mathcal{X}} =& \mathbb{1} + \phi\mathcal{X} + \frac{\phi^2}{2}\mathcal{X}^2 + \frac{\phi^3}{3!}\mathcal{X}^3 + \cdots \\ =& \mathbb{1}\underbrace{\left(1 - \frac{\phi^2}{2} + \frac{\phi^4}{4!} + \cdots\right)}_{=\cos\phi} \\ &+ \mathcal{X}\underbrace{\left(\phi - \frac{\phi^3}{3!} + \frac{\phi^5}{5!} + \cdots\right)}_{=\sin\phi} \end{aligned} \tag{110}$$

Now, looking at Eq. (94) we see that the matrix exponent *a la* (110) is its formal solution:

$$\begin{pmatrix} x(\phi) \\ y(\phi) \\ z(\phi) \end{pmatrix} = e^{\phi\mathcal{M}_z} \begin{pmatrix} x(0) \\ y(0) \\ z(0) \end{pmatrix} = \begin{pmatrix} \cos\phi & -\sin\phi & 0 \\ \sin\phi & \cos\phi & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} x(0) \\ y(0) \\ z(0) \end{pmatrix} \tag{111}$$

We can also check that M_z generates the following trasformations of momenta:

$$\begin{aligned} \dot{p}_x &= [p_x, M_z] = [p_x, (xp_y - yp_x)] = -p_y \\ \dot{p}_y &= [p_y, M_z] = [p_y, (xp_y - yp_x)] = p_x \\ \dot{p}_x &= [p_z, M_z] = [p_z, (xp_y - yp_x)] = 0 \end{aligned} \tag{112}$$

i.e. the transformation M_z acts on $\vec{p}$ alos as a rotation around z-axis

1.6.5 Algebra of rotations and angular momentum

A general element of 3×3 rotation matrix, O is given by the matrix exponent:

$$O = e^{\vec{\alpha}\cdot\vec{\mathcal{M}}} \tag{113}$$

The matrices O preserve the length of the 3-vectors that they rotate, ie.

$$O^T O = \mathbb{1} \tag{114}$$

Their property is such that, if two matrices O_1, O_2 are of the form (113), then their product $O_3 = O_1 O_2$ is also of this form

The matrices $\mathcal{M}_x, \mathcal{M}_y, \mathcal{M}_z$ (95) commute as follows:

$$\mathcal{M}_x\mathcal{M}_y - \mathcal{M}_y\mathcal{M}_x \equiv [\mathcal{M}_x, \mathcal{M}_y] = \mathcal{M}_z \tag{115}$$

or

$$[\mathcal{M}_i, \mathcal{M}_j] = \epsilon_{ijk}\mathcal{M}_k \tag{116}$$

Back to integrals of motion. Let us now find the Poisson bracket of twi components of the angular momenta M_x and M_y. We will see that

$$[M_x, M_y] = M_z \tag{117}$$

similarly to Eq. (115).

where

$$M_i = \epsilon_{ijk} x^j p^k \tag{118}$$

As an exercise, we can do a general commutator between i-th and j-th components of $\vec{M}$. At this step we need to use known identity

$$\varepsilon_{abc}\varepsilon_{adf} = \delta_{bd}\delta_{cf} - \delta_{bf}\delta_{cd} \tag{119}$$

so

$$\varepsilon_{ikl}\varepsilon_{jmk}p_l x_m = \varepsilon_{kli}\varepsilon_{kjm}x_m p_l = (\delta_{lj}\delta_{im} - \delta_{lm}\delta_{ij})x_m p_l = x_i p_j - \vec{x}\cdot\vec{p}\delta_{ij} \tag{120}$$

$$\varepsilon_{ikl}\varepsilon_{jln}x_k p_n = \varepsilon_{lik}\varepsilon_{lnj}x_k p_n = (\delta_{in}\delta_{kj} - \delta_{ij}\delta_{kn})x_k p_n = x_j p_i - \vec{x}\cdot\vec{p}\delta_{ij} \tag{121}$$

subtracting these two results we obtain:

$$[M_i, M_j] = x_i p_j - x_j p_i \tag{122}$$

We see something, that bring to mind thoughts about angular momentum. Let's quite rewrite this answer using identity (119) in another direction:

$$[M_i, M_j] = x_i p_j - x_j p_i = (\delta_{im}\delta_{jn} - \delta_{in}\delta_{jm})x_m p_n = \varepsilon_{kij}\varepsilon_{kmn}x_m p_n = \\ = \varepsilon_{ijk}(\vec{x}\times\vec{p})_k = \varepsilon_{ijk}M_k \tag{123}$$

This is an important general result, that stays true for angular momenta of all types (even for spin in quantum mechanics).

Therefore, we have found the representation of the group of rotations in 3-dimensional space in Hamiltonian mechanics (substituting matrix commutator with the Poisson bracket).

1.7 Canonical transformation

Take any function $F(q,p)$ and introduce new variables

$$\begin{aligned} q' &= [q, F(q,p)] \\ p' &= [p, F(q,p)] \end{aligned} \tag{124}$$

One can check that

$$[q', p'] = [q, p] = 1 \tag{125}$$

Such a transformation is called *canonical transformation*

Then in new variables the Hamilton equations won't change:

$$\begin{aligned} \frac{dq'}{dt} &= \frac{\partial H(q',p')}{\partial p'} \\ \frac{dp'}{dt} &= -\frac{\partial H(q',p')}{\partial q'} \end{aligned} \tag{126}$$

where $H(q',p') = H(q(q',p'), p(q',p'))$.

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