Physical kinetics seminar
2017 11 27

First chapter of Liboff's book is about the Liouville equation, but we first need a reminder on classical mechanics.

1.1 Elements of Classical Mechanics

1.1.1 Generalized coordinates and the Lagrangian

The number of degrees of freedom of a system corresponds to the minimum number of parameters necessary to uniquely specify the location and orientation of the system in physical space.

The independent parameters are called generalized coordinates.

If we have N particles, subject to k constraints, then the number of generalized coordinates is $3N-k$.

So

$$q_i = q_i(\vec{r}_1, \dots, \vec{r}_N, t) \quad , \quad i = 1, \dots 3N-k$$

For now we will forget the real space and just say that we have N degrees of freedom. Then

$$q = (q_1, \dots, q_N)$$

are the generalized coordinates and

$$\dot{q} = (\dot{q}_1, \dots, \dot{q}_N)$$

are the generalized velocities.

We assume that the system is in a conservative ($\vec{F}_j = -\nabla_j V$) potential $V(q)$. The kinetic energy is $T(q, \dot{q})$.

We introduce the Lagrangian of the system

$$L = L(q, \dot{q}) = T(q, \dot{q}) - V(q)$$

In general, the Lagrangian can be time-dependent $\rightarrow L(q, \dot{q}, t)$.

Now we introduce the action integral

$$S = \int_1^2 \mathcal{L}(q, \dot{q}, t)\, dt$$

with 1 and 2 labeling some two fixed points.

According to the Hamilton's principle, the motion of the system is such, that the action is at its extremum value. Thus

$$\delta S = \delta \int_1^2 \mathcal{L}(q, \dot{q}, t)\, dt = 0$$

From this we can obtain the Lagrange's equations:

$$\delta S = \int_1^2 \mathcal{L}(q + \delta q, \dot{q} + \delta \dot{q}, t)\, dt - \int_1^2 \mathcal{L}(q, \dot{q}, t)\, dt =$$

$$= \int_1^2 \left[\mathcal{L}(q, \dot{q}, t) + \sum_i \frac{\partial \mathcal{L}}{\partial q_i} \delta q_i + \sum_i \frac{\partial \mathcal{L}}{\partial \dot{q}_i} \delta \dot{q}_i \right] dt - \int_1^2 \mathcal{L}(q, \dot{q}, t)\, dt =$$

$$= \sum_i \int_1^2 \left[\frac{\partial \mathcal{L}}{\partial q_i} \delta q_i + \frac{d}{dt}\left(\frac{\partial \mathcal{L}}{\partial \dot{q}_i} \delta q_i \right) - \left(\frac{d}{dt} \frac{\partial \mathcal{L}}{\partial \dot{q}_i} \right) \delta q_i \right] dt =$$

$$= \underbrace{\sum_i \left(\frac{\partial \mathcal{L}}{\partial \dot{q}_i} \delta q_i \right) \Big|_1^2}_{\text{is } 0\text{, as the endpoints are fixed}} + \sum_i \int_1^2 \underbrace{\left(\frac{\partial \mathcal{L}}{\partial q_i} - \frac{d}{dt} \frac{\partial \mathcal{L}}{\partial \dot{q}_i} \right)}_{\text{must be zero for arbitrary } \delta q_i} \delta q_i\, dt$$

Thus we obtain

$$\left. \frac{d}{dt} \frac{\partial \mathcal{L}}{\partial \dot{q}_i} - \frac{\partial \mathcal{L}}{\partial q_i} = 0 \quad , \quad i = 1 \dots N \right] \text{ Lagrange's equations}$$

1.1.2 Hamilton's equations

We define canonical momentum conjugate to coordinate q_i by

$$p_i = \frac{\partial \mathcal{L}}{\partial \dot{q}_i}$$

From Lagrange's equations we see that

$$\frac{d}{dt} p_i = \frac{d}{dt} \frac{\partial \mathcal{L}}{\partial \dot{q}_i} = \frac{\partial \mathcal{L}}{\partial q_i}$$

Thus, if coordinate q_i does not appear in the Lagrangian, its conjugate momentum is constant in time. Such coordinates are called cyclic coordinates.

We can change our variables from $(q, \dot{q})$ to (q, p). It is done via Legendre's transformation.

If we have $L = L(q, \dot{q}, t)$, then

$$
\begin{aligned}
dL &= \sum_i \frac{\partial L}{\partial q_i} dq_i + \sum_i \frac{\partial L}{\partial \dot{q}_i} d\dot{q}_i + \frac{\partial L}{\partial t} dt = \\
&= \sum_i \dot{p}_i dq_i + \sum_i p_i d\dot{q}_i + \frac{\partial L}{\partial t} dt = \\
&= \sum_i \dot{p}_i dq_i + \sum_i d(p_i \dot{q}_i) - \sum_i \dot{q}_i dp_i + \frac{\partial L}{\partial t} dt
\end{aligned}
$$

From here

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

We define the Hamiltonian $H = H(q, p, t) = \sum_i p_i \dot{q}_i - L$ and immediately obtain Hamilton's equations:

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

and $\frac{\partial H}{\partial t} = -\frac{\partial L}{\partial t}$.

So if the Hamiltonian does not depend on p_i or q_i, then q_i or p_i are constant.

We can also calculate the time derivative of the Hamiltonian:

$$
\frac{dH}{dt} = \sum_i \frac{\partial H}{\partial q_i} \dot{q}_i + \sum_i \frac{\partial H}{\partial p_i} \dot{p}_i + \frac{\partial H}{\partial t} = -\sum_i \dot{p}_i \dot{q}_i + \sum_i \dot{q}_i \dot{p}_i - \frac{\partial L}{\partial t} = -\frac{\partial L}{\partial t}
$$

If the Lagrangian does not depend on time explicitly, then the Hamiltonian is a constant in time.

Further, if transformation to generalized coordinates is not time-dependent and the ~~forces acting on the~~ potential does not depend on generalized velocities, that is, the forces are conservative, then the Hamiltonian can be identified with total energy.

This is the case for a system of particles with interaction potential depending only on distances.

As an illustration of the Hamiltonian concept I will now do

Exercise 1.2:

Free particle Hamiltonian in spherical coordinates.

$$\mathcal{L} = T = \frac{m}{2}\dot{\vec{r}}^2$$

$$\dot{\vec{r}} = \dot{r}\vec{u}_r + r\dot{\theta}\vec{u}_\theta + r\sin\theta\,\dot{\varphi}\,\vec{u}_\varphi$$

$$\mathcal{L} = \frac{m}{2}\left(\dot{r}^2 + r^2\dot{\theta}^2 + r^2\sin^2\theta\,\dot{\varphi}^2\right)$$

$$p_r = \frac{\partial\mathcal{L}}{\partial\dot{r}} = m\dot{r}, \quad p_\theta = \frac{\partial\mathcal{L}}{\partial\dot{\theta}} = mr^2\dot{\theta}, \quad p_\varphi = \frac{\partial\mathcal{L}}{\partial\dot{\varphi}} = mr^2\sin^2\theta\,\dot{\varphi}$$

$$\Rightarrow \dot{r} = \frac{p_r}{m} \qquad \dot{\theta} = \frac{p_\theta}{mr^2} \qquad \dot{\varphi} = \frac{p_\varphi}{mr^2\sin^2\theta}$$

It is important here that $p_\theta \neq \vec{p}\cdot\vec{n}_\theta$, $p_\varphi \neq \vec{p}\cdot\vec{u}_\varphi$

$$H = \sum_i p_i\dot{q}_i - \mathcal{L} = p_r\dot{r} + p_\theta\dot{\theta} + p_\varphi\dot{\varphi} - \mathcal{L} =$$

$$= \frac{p_r^2}{m} + \frac{p_\theta^2}{mr^2} + \frac{p_\varphi^2}{mr^2\sin^2\theta} - \frac{m}{2}\left(\frac{p_r^2}{m^2} + \frac{p_\theta^2 r^2}{m^2r^4} + \frac{p_\varphi^2 r^2\sin^2\theta}{m^2r^4\sin^4\theta}\right) =$$

$$= \frac{p_r^2}{2m} + \frac{p_\theta^2}{2mr^2} + \frac{p_\varphi^2}{2mr^2\sin^2\theta}$$

So, p_φ is constant momentum, while in Cartesian coordinates all three p_i are conserved.

— — —

Now we can discuss a few more example Hamiltonians.

An electrodynamic Hamiltonian describes a particle of mass m and charge e that moves in an electromagnetic field with vector potential $\vec{A}$ and scalar potential ~~φ~~ ϕ:

$$H = \frac{1}{2m}\left(\vec{p} - \frac{e}{c}\vec{A}\right)^2 + e\phi \quad \Big| \quad H = \frac{1}{2m}\left(\vec{p} - e\vec{A}\right)^2 + e\phi \text{ in SI}$$

$$\vec{p} = m\vec{v} + \frac{e}{c}\vec{A}$$

The electric and magnetic fields are expressed using the potentials as

$$\vec{\mathcal{E}} = -\nabla\phi - \frac{1}{c}\frac{\partial\vec{A}}{\partial t} \quad \Big| \quad \vec{\mathcal{E}} = -\nabla\phi - \frac{\partial\vec{A}}{\partial t} \text{ in SI}$$

$$\vec{B} = [\nabla\times\vec{A}]$$

Gauge transformations

$$\phi \to \phi' - \frac{1}{c}\frac{\partial\chi}{\partial t}$$

$$\vec{A} \to \vec{A}' + \nabla\chi$$

leave electric and magnetic field invariant.

$$\phi \to \phi' = \phi - \frac{\partial\chi}{\partial t} \text{ in SI}$$

From Hamilton's equation we can obtain the Lorentz force

$$\vec{F} = e\left(\vec{\mathcal{E}} + \left[\frac{\vec{v}}{c}\times\vec{B}\right]\right) \quad \Big| \quad \vec{F} = e\left(\vec{\mathcal{E}} + [\vec{v}\times\vec{B}]\right) \text{ in SI}$$

Note that all this is written in Gaussian unit system.

There is a rather lengthy exercise concerning this Hamiltonian.

Another example is the Relativistic one particle Hamiltonian

$$H = \sqrt{p^2 c^2 + m^2 c^4} + V(\vec{r})$$

with relativistic momentum being

$$\vec{p} = \gamma m \vec{v}, \quad \gamma^2 = \frac{1}{1-\beta^2}, \quad \beta = \frac{v}{c}$$

1.1.3 Constants of motion

Function $W = W(q, p, t)$ is called a constant of motion, an integral of the system, or an integral of motion if it remains constant throughout the time as the system undergoes motion.

Formally, there are $2N$ constants of motion, as can be deducted from the number of initial conditions required for the Hamilton's equations. Thus $2N$ constants $\{q_i(0), p_i(0)\}$ specify the state of the system. Now we turn to the geometric interpretation of this.

In $2N+1$-dimensional space, $2N$ surfaces define a curve. This is logical, as a surface is defined by a function of coordinates being equal to a constant, and $2N+1$ constants would specify a point.

So, in 3-space we could define surfaces by

$$f(x, y, z) = C_1$$
$$g(x, y, z) = C_2$$

Together these two surfaces define a curve, which can be written in parametric form as

$$x = x(t) \qquad y = y(t) \qquad z = z(t)$$

Before we go further, we need to introduce Γ-space.

1.1.4 Γ-space

For a system with N degrees of freedom, Γ-space is a 2N-dimensional Cartesian space whose axes are the $\{q_i, p_i\}$ variables.

The state of a system ~~at a~~ at a given time moment is a single point in Γ-space.

Consider a harmonic oscillator $H = \frac{p^2}{2m} + \frac{1}{2}kq^2 = E = \text{const}$

From here

$$\frac{p^2}{2mE} + \frac{q^2}{2\frac{E}{k}} = 1 \Rightarrow \left(\frac{q}{a}\right)^2 + \left(\frac{p}{b}\right)^2 = 1$$

We get an equation for the orbit. It is an ellipse in Γ-space.
We see that at any time the state of the system (q, p) is on an ellipse in Γ-space, but we cannot say where exactly. Thus we see that time is suppressed in Γ-space.

Time is included explicitly in 2N+1 $\tilde{\Gamma}$-space, which has an additional orthogonal time axis, if compared to Γ-space.

The system trajectory (or dysfunctional orbit...)

$$[q_i(t), p_i(t)]$$

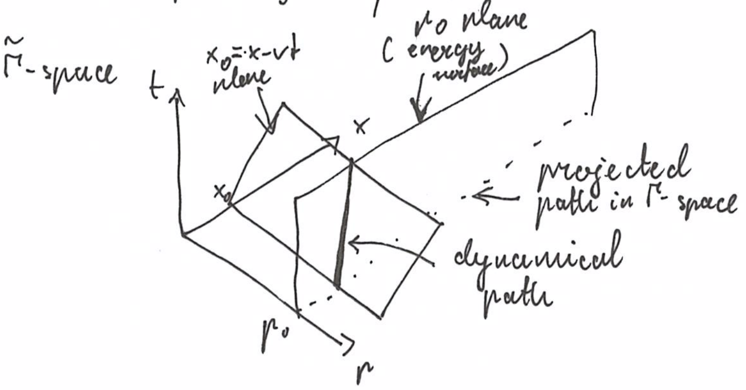
is a curve in $\tilde{\Gamma}$-space.

A constant of motion $W_1(q, p, t) = C_1$ defines a surface in $\tilde{\Gamma}$-space.
An intersection of 2N such independent surfaces $W_1, \dots, W_{2N}$ determines a curve in $\tilde{\Gamma}$-space, which is the system trajectory

$$q_i = q_i(y) \quad , \quad p_i = p_i(y) \quad , \quad t = t(y)$$

So, again, 2N constants determine the system trajectory.
If we are interested in the projected motion in Γ-space, it is determined by 2N-1 constants.

Example - free particle motion in one dimension



$$x_0 = x - vt$$
$$p_0 = p = mv$$
$$x = x_0 + \frac{p_0}{m} t$$

1.1.5 Dynamic reversibility

We consider a system, which is described by a Hamiltonian, which is invariant under time reversal $\Rightarrow H(t) = H(-t)$.

If $\{q(t), p(t)\}$ is a solution of the Hamilton's equations, then another solution is $\{q(-t), -p(-t)\}$.

To prove this, we remember Hamilton's equations

$$\frac{dq}{dt} = \frac{\partial H}{\partial p} \quad , \quad \frac{dp}{dt} = -\frac{\partial H}{\partial q}$$

Now we set $t' = -t$, thus

$$-\frac{dq}{dt'} = \frac{\partial H}{\partial p} \quad , \quad -\frac{dp}{dt'} = -\frac{\partial H}{\partial q}$$

The equations regain the same form if $q' = q$, $p' = -p$.

Physically, this means that if a particle goes from point 1 to point 2 along some trajectory, then it could have gone from point 2 to point 1 along the same trajectory.

1.1.6 Equations of Motion for Dynamic Variables

We assume that $u = u(q, p, t)$ is some dynamic variable of interest. Its time derivative is

$$\frac{du}{dt} = \sum_i \left(\frac{\partial u}{\partial q_i} \dot{q}_i + \frac{\partial u}{\partial p_i} \dot{p}_i \right) + \frac{\partial u}{\partial t}$$

We can use Hamilton's equations to write this as

$$\frac{du}{dt} = \sum_i \left(\frac{\partial u}{\partial q_i} \frac{\partial H}{\partial p_i} - \frac{\partial u}{\partial p_i} \frac{\partial H}{\partial q_i} \right) + \frac{\partial u}{\partial t}$$

Now we introduce the Poisson bracket as

$$[A, B] = \sum_i \left(\frac{\partial A}{\partial q_i} \frac{\partial B}{\partial p_i} - \frac{\partial B}{\partial q_i} \frac{\partial A}{\partial p_i} \right)$$

Then

$$\frac{du}{dt} = [u, H] + \frac{\partial u}{\partial t}$$

This is the equation of motion for the dynamical variable $u(q, p, t)$.

We have the following properties of Poisson brackets:

$$[A, B] = -[B, A]$$

$$[A, c] = 0 \quad , \text{ if } c \text{ is a constant}$$

$$[AB, F] = A[B, F] + [A, F]B$$

$$[A, [B, F]] + [B, [F, A]] + [F, [A, B]] = 0 \qquad / \text{ Jacobi's identity}$$

$$\frac{\partial}{\partial t}[A, B] = \left[\frac{\partial A}{\partial t}, B\right] + \left[A, \frac{\partial B}{\partial t}\right]$$

$$[A, B(A)] = 0 \qquad / \text{ assuming } B(A) \text{ has Taylor series}$$

If u does not depend explicitly on time, then $\frac{du}{dt} = [u, H]$.

If also $u = u(H)$, then $\frac{du}{dt} = 0 \Rightarrow$ Any dynamic variable that is function only of the Hamiltonian is a constant of motion.

We can use the Poisson brackets to rewrite Hamilton's equations as

$$\dot{q}_i = [q_i, H] \quad , \quad \dot{p}_i = [p_i, H]$$

We also have fundamental Poisson bracket relations

$$[q_i, q_j] = 0, \quad [p_i, p_j] = 0 \quad , \quad [q_i, p_j] = \delta_{ij}$$