Lagrangian and Hamiltonian Mechanics

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1 Lagrangian and Hamiltonian formalism

1.1 The principle of extremum action

Newtonian formalism describes a mechanical system as a differential equation and thus is local in time. In Lagrangian formalism, we assume that we are given two times t_1 and t_2 with a particle being at the position x_1 and x_2 respectively, the path of the system on the configuration space is the one that extremizes the action

$$
\begin{aligned}
S &= \int_{t_1}^{t_2} L\left(x,\dot{x},t\right)dt. \\
0 = \delta S &= \int_{t_1}^{t_2} \delta L\left(x,\dot{x},t\right)dt \\
&= \int \left(\frac{\partial L}{\partial x}\delta x + \frac{\partial L}{\partial \dot{x}}\underbrace{\delta \dot{x}}_{d(\delta x)/dt} + \frac{\partial L}{\partial t}\underbrace{\delta t}_{0}\right)dt \\
&= \int \left(\frac{\partial L}{\partial x}\delta x + \frac{\partial L}{\partial \dot{x}}\frac{d}{dt}\delta x\right)dt
\end{aligned}
$$

Using integration by path, the second term on the RHS can be expressed as

$$
\int dt \frac{\partial L}{\partial \dot{x}}\frac{d}{dt}\delta x = \underbrace{\delta x \frac{\partial L}{\partial \dot{x}}\bigg|_{t_1}^{t_2}}_{0} - \int \frac{d}{dt}\frac{\partial L}{\partial x}\delta x dt
$$

where the first term vanishes because the end points are fixed. Therefore,

$$0 = \int \left(\frac{\partial L}{\partial x} - \frac{d}{dt}\frac{\partial L}{\partial x} \right) \delta x dt.$$

It can be shown that this implies the Euler-Lagrange equation

$$\boxed{\frac{\partial L}{\partial x} - \frac{d}{dt}\frac{\partial L}{\partial x} = 0}.$$

For a conservative force field, $L = T - U$ leads to the familiar equation of motion $m\ddot{x} = -\frac{\partial U}{\partial x}$. For nonconservative force field, the Euler-Lagrange equation can be modified to take into account the nonconservative force by separating the generalized force Q into the conservative and nonconservative parts

$$Q = -\frac{\partial U(q)}{\partial q} + Q_{\text{nc}}.$$

Then

$$\begin{aligned} \frac{d}{dt}\frac{\partial T}{\partial \dot{q}} - \frac{\partial T}{\partial q} &= Q \\ \implies \frac{d}{dt}\frac{\partial L}{\partial \dot{q}} - \frac{\partial L}{\partial q} &= Q_{\text{nc}}. \end{aligned}$$

1.2 Legendre transform

A puzzle: given a function $f(x)$, let $\left.\frac{df}{dx}\right|_{x_0} = \phi$. Can we find a function $G(\phi)$ such that $\frac{dG}{d\phi} = x$?

If $f(x) = ax^n$, then $G(\phi) = F(x(\phi))$ works since $\frac{dG}{d\phi} = \frac{df}{dx}\frac{dx}{d\phi} = \phi\frac{dx}{d\phi} = \phi\frac{d}{d\phi}\left(\frac{\phi}{an}\right)^{\frac{1}{n-1}} \propto x$. Note that we have to invert $\phi(x)$ to find $x(\phi)$. The general recipe for any function of x is the *Legendre transform*

$$\boxed{G(\phi) = -\phi x(\phi) - F(x(\phi))}$$

since

$$\frac{dG}{d\phi} = x(\phi) + \phi\frac{dx}{d\phi} - \phi\frac{dx}{d\phi} = x.$$

Geometrically, $-G(\phi)$ is the intercept of the tangent of f at a point x_0 with the $x = 0$ axis.

At x_0,

$$\begin{aligned} y - F(x_0) &= \left.\frac{dF}{dx}\right|_{x_0} (\overbrace{x}^{0} - x_0) \\ y &= F(x_0) - \phi x. \end{aligned}$$

Example. $f(x, y) = \frac{ax^2}{2} + \frac{by^2}{2} + cxy$. Then the process of finding $G(\phi, y)$ is the same given that y is hold constant at all time.

1.3 Hamiltonian

Gievn a Lagrangian L, the momentum p canonically conjugated to a coordinate q is defined by

$$p\left(q,\dot{q},t\right)\equiv\frac{\partial L\left(q,\dot{q},t\right)}{\partial\dot{q}}.$$

Substitute this into the Euler-Lagrange equation gives

$$\dot{p}\left(q,\dot{q},t\right)=\frac{\partial L\left(q,\dot{q},t\right)}{\partial q}.$$

Inverting the functions of $\dot{q}$ to functions of p gives the Hamilton's equations of motion.

Example. A harmonic oscillator $L=\frac{1}{2}m\dot{q}^2-\frac{1}{2}kq^2$.

$$\begin{aligned}p=\frac{\partial L}{\partial\dot{q}}=m\dot{q}&\iff\dot{q}=\frac{p}{m},\\ \dot{p}=\frac{\partial L}{\partial q}&\iff\dot{p}=-kq.\end{aligned}$$

To do this systematically, define H to be the Legendre transform of L: $H(p,q,t)=p\dot{q}-L$. Then the Hamilton's equation of motion are

$$\boxed{\dot{q}=\frac{\partial H}{\partial p},\ \dot{p}=-\frac{\partial H}{\partial q}}$$

For the harmonic oscillator,

$$\begin{aligned}H&=\frac{p^2}{2m}+\frac{kq^2}{2}\\ \implies\ddot{p}+\omega^2p&=0\\ \implies p(t)&=p(0)\cos(\omega t)-\frac{kq(0)}{\omega}\sin(\omega t),\\ q(t)&=q(0)\cos(\omega t)+\frac{p(0)}{m\omega}\sin(\omega t).\end{aligned}$$

By defining $Q=q(km)^{\frac{1}{4}}$ and $P=\frac{p}{(km)^{\frac{1}{4}}}$, the conservation of energy takes on a very simple form

$$Q^2+P^2=\frac{2E}{\omega},$$

where the trajectory in phase space is a circle with radius $\sqrt{\frac{2E}{\omega}}$. Notice that we have eliminated q first to get the equation of motion for p. The Hamiltonian treats q and p symmetrically.

1.4 Constants of motion

Suppose that $\frac{df(q,p,t)}{dt}$ is a constant, then

$$\begin{aligned}0=\frac{df(q,p,t)}{dt}&=\frac{\partial f}{\partial q}\dot{q}+\frac{\partial f}{\partial p}\dot{p}+\frac{\partial f}{\partial t}\\ &=\underbrace{\left(\frac{\partial f}{\partial q}\frac{\partial H}{\partial p}-\frac{\partial f}{\partial p}\frac{\partial H}{\partial q}\right)}_{\{f,H\}}+\frac{\partial f}{\partial t}\end{aligned}$$

Useful identities for Poisson brackets:

$$\{f, gh\} = g\{f, h\} + \{f, g\} h.$$
$$\{\{f, g\}, h\} = \{\{h, f\}, g\} = \{\{g, h\}, f\}.$$

Example. $H = \frac{p^2}{2m} - kq$.

Consider an apparently contrived function $f = q - \frac{p}{m}t + \frac{k}{2m}t^2$. It is a constant of motion;

$$\frac{df}{dt} = \{f, H\} + \frac{\partial f}{\partial t} = \frac{p}{m} - \left(-\frac{t}{m}\right)(-k) - \frac{p}{m} + \frac{kt}{m} = 0.$$

Consider another function $g = p - kt$. It is also a constant of motion;

$$\frac{dg}{dt} = \{g, H\} + \frac{\partial g}{\partial t} = 0 \cdot \frac{\partial H}{\partial p} - (-k) - k = 0.$$

In fact, f and g are nothing but initial conditions $q(0)$ and $p(0)$ respectively. These are called *trajectory constants*. Any constant of motion is a combination of trajectory constans. Thus, there always exist $2n$ constants of motion whether H depends explicitly on time or not.

Example. A free particle $H = \frac{p^2}{2m}$. q is a *cyclic coordinate*, i.e. q is absent from the Hamiltonian $\Longrightarrow p = -\frac{\partial H}{\partial q}$ is conserved.

Example. $H = p_1\left(\frac{p_2}{m} - \gamma q_1\right)$. There is no q_2 in the Hamiltonian, so p_2 is a constant.

$$\dot{q}_1 = \frac{\partial H}{\partial p_1} = \frac{p_2(0)}{m} - \gamma q_1$$
$$\Longrightarrow q_1(t) = q(0)e^{-\gamma t} + \frac{p_2(0)}{m}\frac{1 - e^{\gamma t}}{\gamma}.$$

Example. $H = p_1\left(\frac{p_2}{m} - \gamma q_1\right) + m\omega^2 q_1 q_2$.

$$\dot{p}_2 = -\frac{\partial H}{\partial q_2} = -m\omega^2 q_1$$
$$\dot{q}_1 = \frac{\partial H}{\partial p_1} = \frac{p_2}{m} - \gamma q_1$$
$$\Longrightarrow \boxed{\ddot{q}_1 + \gamma\dot{q}_1 + m\omega q_1 = 0}.$$

We have obtained the equation of motion of a damped harmonic oscillator even though there is no explicit time dependence in the Hamiltonian!

Example. A rotor with two particle with masses m_1 and m_2 and the reduced mass $\mu = \frac{m_1 m_2}{m_1 + m_2}$ and the Lagrangian

$$L = \frac{\mu}{2}\left[\dot{r}^2 + \left(r\dot{\theta}\right)^2 + \left(r\sin\theta\dot{\phi}\right)^2\right] - U(r).$$

p_r is the momentum and p_θ is the angular momentum. But it is not obvious by looking at $p_\phi = \frac{\partial L}{\partial \dot{\phi}} = \mu r^2 \sin^2\theta\dot{\phi}$ whether p_ϕ is a constant of motion or not. We can write down the Hamiltonian

$$H = p_r\dot{r} + p_\theta\dot{\theta} + p_\phi\dot{\phi} - L$$
$$= \frac{p_r^2}{2\mu} + \frac{p_\theta^2}{2\mu r^2} + \frac{p_\phi^2}{2\mu r^2 \sin^2\theta} + U(r).$$

Consider

$$\begin{aligned} p_\theta \dot{p}_\theta &= p_\phi^2 \frac{\cos\theta}{\sin^2\theta}\dot{\theta} \\ \frac{1}{2}\frac{d}{dt}\left(p_\theta^2\right) &= -\frac{1}{2}p_\phi^2 \frac{d}{dt}\frac{1}{\sin^2\theta} \\ \implies p_\theta^2 + \frac{p_\phi^2}{\sin^2\theta} &\equiv L^2 = \text{constant.} \end{aligned}$$

Using what we just found out, the Hamiltonian can be written in the familiar form (as seen in quantum mechanics, for example)

$$\boxed{H = \frac{p_r^2}{2\mu} + \frac{L^2}{2\mu r^2} + U(r)}$$

1.5 When the Hamiltonian is not the energy

Suppose that $L = L(q, \dot{q})$. Then

$$\begin{aligned} \frac{dL}{dt} &= \frac{\partial L}{\partial q}\dot{q} + \frac{\partial L}{\partial \dot{q}}\ddot{q} \\ &= \frac{d}{dt}\frac{\partial L}{\partial \dot{q}}\dot{q} + \frac{\partial L}{\partial \dot{q}}\ddot{q} \text{ (cancellation of dots)} \\ 0 &= \frac{d}{dt}\boxed{\underbrace{\left(\dot{q}\frac{\partial L}{\partial \dot{q}} - L\right)}_{H}}, \end{aligned}$$

where H is the Hamiltonian. This shows that H is a constant of motion, and usually we think of H as the energy. The question is then whether H is actually the energy. And the answer is "not always."

To demonstrate this point, suppose that $T = \sum \frac{1}{2}m\dot{x}_i^2$, that $x = x(q)$, that is, x is a function of generalized coordinates alone (and not generalized velocity or time), with the change-of-coordinates matrix A, and that the force is conservative. Then the kinetic energy is of the quadratic form

$$T = \sum_{j,k} A_{jk}\dot{q}_j\dot{q}_k,$$

where $\frac{1}{2}m$ is absorbed into A. The hamiltonian is

$$H = \sum \dot{q}_i \frac{\partial T}{\partial \dot{q}_i} - T + U.$$

$\frac{\partial T}{\partial q_i} = \sum_k A_{ik}\dot{q} + \sum_j A_{ij}\dot{q}_j \implies \sum \dot{q}_i \frac{\partial T}{\partial q_i} = 2T;$

$$H = T + U.$$

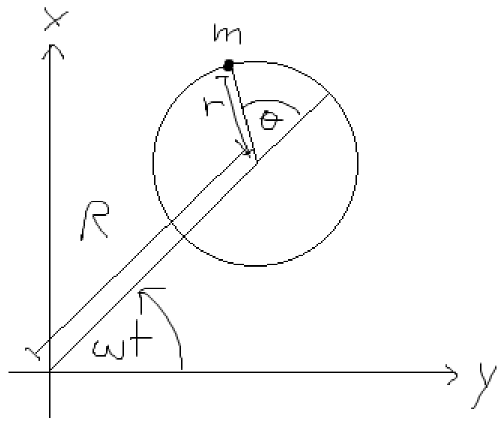
We see that in this example, the Hamiltonian is the energy only because

$$\frac{\partial L}{\partial t} = 0, \tag{1}$$

$$U = U(q), \tag{2}$$

$$T = T(q) \text{ is quadratic.} \tag{3}$$

Example. Consider a planar system with a bead confined to move only along a hoop of radius r whose center is attached to the end of a stick of length R. The stick is rotated with a constant angular velocity ω as shown in the picture. There is no gravity.



$$
\begin{aligned}
(x, y) &= (R\cos(\omega t) + r\cos(\omega t + \theta), R\sin(\omega t) + r\sin(\omega t + \theta)) \\
\implies T &= \frac{1}{2}m\left[R^2\omega^2 + r^2(\omega + \theta)^2 + 2R\omega\left(\omega + \dot{\theta}\right)\cos\theta\right]
\end{aligned}
$$

$$
\implies \ddot{\theta} + \frac{\omega^2 R}{r}\sin\theta = 0,
$$

which is the equation of motion of the physical pendulum even if there is no gravity here. The reason is that an observer sitting at the end of the stick would feel a fictitious centrifugal force outward having the magnitude of $m\omega^2 R\sin\theta$.

Another important observation is that H is not the energy since apparently T is not quadratic. $\frac{\partial H}{\partial t} = 0$, but the energy $\frac{1}{2}I\omega^2$ is not conserved since to keep the angular momentum L constant while ω is also constant, the moment of inertia I has to vary in time.

1.6 Liouvillian

Define the Liouvillian $\mathcal{L} = \left(\frac{\partial H}{\partial p}\frac{\partial}{\partial q} - \frac{\partial H}{\partial q}\frac{\partial}{\partial p}\right)$. Then the Hamilton's equations of motion become

$$
\dot{p} = \mathcal{L}(p), \dot{q} = \mathcal{L}(q).
$$

Now we can write the time evolution of a Hamiltonian system in terms of a linear map that maps the initial $q(0)$ and $p(0)$ to $q(t)$ and $p(t)$ at later times analogous to the time evolution by a unitary in quantum mechanics.

$$\begin{aligned}
q(t) &= q(0) + \int_0^t dt' \mathcal{L}\left(t'\right) q\left(t'\right) \\
&= q(0) + \int_0^t dt' \mathcal{L}\left(t'\right) \left(q(0) + \int_0^{t'} dt'' \mathcal{L}\left(t''\right) q\left(t''\right)\right) + \ldots \\
&= \left[1 + \underbrace{\int_0^t dt' \mathcal{L}\left(t'\right)}_{\mathcal{L}} + \underbrace{\int_0^t dt' \mathcal{L}\left(t'\right) \int_0^{t'} dt'' \mathcal{L}\left(t''\right)}_{\frac{t^2}{2!}\mathcal{L}^2} + \ldots\right] q(0) \\
&= e^{\mathcal{L}t} q(0),
\end{aligned}$$

and similarly,

$$p(t) = e^{\mathcal{L}t} p(0).$$

Example. $H = \frac{p^2}{2m} - kq$.

$$\mathcal{L} = \frac{p}{m}\frac{\partial}{\partial q} + k\frac{\partial}{\partial p}.$$

$\mathcal{L}(p) = k$, $\mathcal{L}^2(p) = \mathcal{L}\left(\mathcal{L}(p)\right) = \mathcal{L}k = 0$. So the series terminates and we get that

$$p(t) = e^{\mathcal{L}t}(p)\Big|_0 = p(0) + kt.$$

$\mathcal{L}(q) = \frac{p}{m}$, $\mathcal{L}^2(q) = \frac{k}{m}$, $\mathcal{L}^3(q) = 0$. So

$$q(t) = e^{\mathcal{L}t}(q)\Big|_0 = q(0) + \frac{p(0)}{m}t + \frac{k}{2m}t^2.$$

We can go further and write the Liouvillian as a superoperator similar to the time evolution $A(t) = U^\dagger A(0) U$ of an operator A in the Heisenberg picture.

1.7 Coordinate transformation

A mass on a spring is attached to a car moving with velocity v such that $H = \frac{p^2}{2m} + \frac{1}{2}k(x - vt)^2$. Suppose that we want to simplify the problem by going into the moving frame and define $X = x - vt$. What is the conjugate momentum P?

Go back to the Lagrangian;

$$\begin{aligned}
L &= \frac{1}{2}m\dot{x}^2 - \frac{1}{2}k(x - vt)^2 \\
X &= x - vt \\
\dot{X} &= \dot{x} - v.
\end{aligned}$$

The new Lagrangian is

$$\tilde{L} = \frac{1}{2}m\left(\dot{X} + v\right)^2 - \frac{1}{2}kX^2.$$

The new momentum is

$$P = \frac{\partial \tilde{L}}{\partial \dot{X}} = m\left(\dot{X} + v\right).$$

Then

$$\tilde{H} = P\dot{X} - \tilde{L} = \frac{(P - mv)^2}{2m} + \frac{1}{2}kX^2 - \underbrace{\frac{1}{2}mv^2}_{\text{constant}}.$$

Without going back to the Lagrangian, we might be tempt to simply write

$$\begin{aligned} P = m\dot{X} &= p - mv \\ \implies \frac{p^2}{2m} &= \frac{(P + mv)^2}{2m}. \end{aligned}$$

But that would be off by a sign.

1.7.1 Action Principle for the Hamiltonian

In searching for a set of transformations that preserve Hamilton's equations of motion, we go back to the action principle. Can the action principle be formulated in terms of the Hamiltonian alone? The answer is yes. Let the action be

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

$$0 = \delta S = \int_{t_1}^{t_2} dt \left(\delta p \dot{q} + \underbrace{p\delta\dot{q}}_{\frac{d}{dt}(p\delta q) - \dot{p}\delta q} - \frac{\partial H}{\partial q}\delta q - \frac{\partial H}{\partial p}\delta p \right).$$

Assume that δq and δp are varied independently.

$$0 = \underbrace{p\,\delta q\Big|_{t_1}^{t_2}}_{0} + \int_{t_1}^{t_2} dt \left(\delta p \left(\dot{q} - \frac{\partial H}{\partial p} \right) - \left(\dot{p} + \frac{\partial H}{\partial q} \right) \delta q \right).$$

The demand that the action is extremized is equivalent to Hamilton's equations

$$\begin{aligned} \dot{q} - \frac{\partial H}{\partial p} &= 0, \\ \dot{p} + \frac{\partial H}{\partial q} &= 0. \end{aligned}$$

Curiously, this does not required the variation in the nomentum at the end points to vanish, although we will assume that from now on. Then for any scalar function $F(q,p,t)$, the action can be modified

$$S = \int_{t_1}^{t_2} dt \left(p\dot{q} - H(q,p,t) + \frac{dF}{dt} \right).$$

1.7.2 Canonical transformations

It is clear from the previous section that for any new Hamiltonian $\mathcal{H}(Q, P, T)$ to give Hamilton's equations, we need

$$\begin{aligned} dt\,(p\dot{q} - H(q,p,t)) &= dt\left(P\dot{Q} - \mathcal{H}(Q,P,t) + \frac{dF(q,p,Q,P,t)}{dt}\right) \\ pdq - Hdt - PdQ &= \mathcal{H}dt + dF, \end{aligned}$$

where $F(q, p, Q, P, t)$ is the *generating function* for a canonical transformation (preserving Hamilton's equations).

We define four types of transformations:
Type 1: $F = F(q, Q)$
Type 2: $F = F(q, P)$
Type 3: $F = F(p, Q)$
Type 4: $F = F(p, P)$
Example. For type 1 transformation $F = qQ$,

$$pdq - Hdt - PdQ = \mathcal{H}dt + \frac{\partial F}{\partial q}dq + \frac{\partial F}{\partial Q}dQ = \mathcal{H}dt + Qdq + qdQ$$

$$\implies \begin{cases} q &= -P, \\ p &= Q. \end{cases}$$

Example. A type 1 transformation of a harmonic oscillator $H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 q^2$. It would be nice if we could transform the Hamiltonian such that it has no Q dependence. That is,

$$H = \frac{f^2(p)}{2m}.$$

We therefore consider this transformation

$$\begin{aligned} p &= f(p)\sin Q, \\ q &= \frac{f(p)}{m\omega}\cos Q, \end{aligned}$$

and find the generating function F.

$$\begin{aligned} \frac{p}{q} &= m\omega \tan Q \\ p = \left(\frac{\partial F}{\partial q}\right)_Q &= m\omega q \tan Q \\ \implies F &= \frac{m\omega q^2}{2}\tan Q + g(Q) \end{aligned}$$

Choose $g(Q) = 0$. Then

$$\begin{aligned} P = -\left(\frac{\partial F}{\partial Q}\right)_q &= -\frac{m\omega q^2}{2}\sec^2 Q \\ &= -\frac{f^2(p)}{2m\omega}\cos^2 Q \sec^2 Q \\ \implies f(p) &= i\sqrt{2m\omega P} \end{aligned}$$

$$\implies \boxed{H = -\omega P}.$$

The Hamiltonian becomes that of the free particle with $P = P(0)$ and $Q = Q(0) - \omega t$! Say, in the study of fluctuation-dissipation relation, if you want to phenomenologically put friction in the system, it is much easier to put friction in at this level after you have transformed the oscillator into a free particle.

Example. A type 2 transformation of a harmonic oscillator $H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 q^2$.

Let P be the "ladder operators."

$$P = \frac{p + im\omega q}{\sqrt{2}}$$

Look for $F(q, P)$.

$$\begin{aligned} pdq - Hdt + QdP &= \mathcal{H}dt + \frac{\partial F}{\partial q}dq + \frac{\partial F}{\partial P}dP \\ p = \left(\frac{\partial F}{\partial q}\right)_P &= \sqrt{2}P - im\omega q \\ &\implies F = \sqrt{2}Pq - \frac{im\omega q^2}{2} + g(P) \\ Q = \left(\frac{\partial F}{\partial P}\right)_q &= \sqrt{2}q + g^{'}(P). \end{aligned}$$

Choose $g^{'}(P) = \frac{iP}{m\omega}$. Then

$$Q = \sqrt{2}q + \frac{iP}{m\omega} = \sqrt{2}q + \frac{i}{m\omega}\left(\frac{p + im\omega q}{\sqrt{2}}\right) = \sqrt{2}q + \frac{ip}{\sqrt{2}m\omega} - \frac{q}{\sqrt{2}} = \frac{q + \frac{ip}{m\omega}}{\sqrt{2}}.$$

(This is wrong but it was from the lecture. Anyway, assuming the result, the Hamiltonian is)

$$\boxed{\mathcal{H} = i\omega PQ},$$

which is the analog of $H = \omega a^\dagger a$ in quantum mechanics, and P and Q, like the ladder operators, evolve trivially in time.

$$P(t) = P(0)e^{-i\omega t}, Q(t) = Q(0)e^{i\omega t}.$$