Lecture 12 - Hamiltonian Mechanics and Phase Space

Lagrangian mechanics have some advantages over Newtonian mechanics such as easier coordinate transforms and the ability to more easily incorporate constraints. However, statistical mechanics is usually expressed in terms of Hamiltonian mechanics. I will first explain the equations and then provide some perspective on why it is used and what it has to do with phase space.

A. Hamiltonian's Equations

In Hamiltonian mechanics, we work with generalized coordinates again. However, a key difference is that we use a generalized momentum p_i, rather than a generalized velocity. The generalized momentum is defined in terms of the Lagrangian:

$$p_i = \frac{\partial L}{\partial \dot{q}_i} \qquad i = 1, 2, \ldots, 3N$$

Note the change in indexing from Lagrangian Mechanics. We are "flattening" the 2D array to 1D.

What is the generalized momentum? Just like we have the gen. coordinate and gen. velocity, this provides a definition of a momentum that is invariant to coordinate transformations. It makes our life easier with different coordinate systems. With this new coordinate (that replaces $\dot{q}_i$), we can define a new quantity called the Hamiltonian by a Legendre transform of the Lagrangian:

$$H(q_i, p_i, t) = \sum_i \dot{q}_i p_i - L(q_i, \dot{q}_i, t) \qquad (1)$$

What is the Hamiltonian and what does it mean? It is usually the total energy (except in rare circumstances).

When is the Hamiltonian equal to the Energy?
(1) the coordinate transform is time independent
(2) the potential is velocity independent

Demonstration that H is the total energy

$$L = K(\dot{q}) - U(q)$$ Assume cartesian, 1D

$$L = \frac{1}{2}mv^2 - U \qquad p = \frac{\partial L}{\partial \dot{q}} = \frac{\partial L}{\partial v} = mv$$ conventional definition of momentum

$$H = \dot{q}p - L$$
$$= vp - L = v \cdot mv - \frac{1}{2}mv^2 + U = \frac{1}{2}mv^2 + U$$
$$\boxed{H = K + U}$$

Using the total derivative dH, the derivative of equation (1), and the Euler Lagrange equation gives Hamilton's equations,

$$\boxed{\frac{dq_i}{dt} = \frac{\partial H}{\partial p_i}, \qquad \frac{dp_i}{dt} = -\frac{\partial H}{\partial q_i}}$$

Two 1^{st} order ODEs instead of one 2^{nd} order ODE.

B. The Poisson Bracket

It is often the case in stat mech that we have quantities that are functions of the p_i and q_i (e.g. pressure). We can use Hamilton's equations to describe the dynamics of these quantities too.

Consider a quantity f that is a function of the p_i, q_i and time,

$$f = f(q_i, p_i, t) \qquad i = 1, 2, \dots, 3N$$

The total derivative of f is given by

$$\frac{df}{dt} = \frac{\partial f}{\partial t} + \sum_{i=1}^{3N} \left(\frac{\partial f}{\partial q_i}\frac{dq_i}{dt} + \frac{\partial f}{\partial p_i}\frac{dp_i}{dt} \right)$$

$\frac{df}{dt}$: total change as f moves through phase space

$\frac{\partial f}{\partial t}$: change of f at one point in phase space.

Now, using Hamilton's equations

$$\frac{dq_i}{dt} = \frac{\partial H}{\partial p_i} \quad , \quad \frac{\partial p_i}{\partial t} = -\frac{\partial H}{\partial q_i}$$

$$\frac{df}{dt} = \frac{\partial f}{\partial t} + \sum_{i=1}^{3N} \left(\frac{\partial f}{\partial q_i}\frac{\partial H}{\partial p_i} - \frac{\partial f}{\partial p_i}\frac{\partial H}{\partial q_i} \right)$$

analogous to the material derivative. How does f change as it is convected through phase space?

There is a compact way of writing the sum on the right-hand side. It is called a Poisson bracket

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

equation of motion of f.

$$\{A, B\} = \sum_{i=1}^{3N} \left(\frac{\partial A}{\partial q_i}\frac{\partial B}{\partial p_i} - \frac{\partial A}{\partial p_i}\frac{\partial B}{\partial q_i} \right) .$$

Why use Hamilton's E.O.M rather than Newton or Lagrange?

(1) Like Lagrange, better coordinate transforms than Newton's E.O.M.

(2) Two 1st order ODEs can sometimes make life easier especially when numerically integrating.

The real value of Hamiltonian mechanics is conceptual, rather than practical.

C. Key Concept 1: Symplectic Geometry

Let us call the 6N-dimensional space (where N is the number of particles) defined by the Lagrangian variables q_i and $\dot{q}_i$ state space. In addition, let us call the 6N-dimensional space defined by the Hamiltonian canonical variables q and p phase space.

Phase space has an important property that state space is not guaranteed to have. Phase space has a symplectic geometry. A symplectic geometry means that the volume of phase space doesn't change with time. The space is incompressible.

A perhaps simplistic way to think about this is that

$$\int dq_1 dq_2 \ldots dq_{3N} dp_1 dp_2 \ldots dp_{3N} = \text{const}$$

guaranteed for p_i but not for $\dot{q}_i$.

This is a critical mathematical property, because it allows us to define a probability density. If phase space changed volume, then we could not normalize probabilities.

Another way to think about this is that p_i are the "proper" variables. They are the correct "conjugate" variable to q.

Show Python Example with symplectic and non-symplectic system.

There is an important theorem for statistical thermodynamics that results from this property. Suppose that $\rho = \rho(q_i, p_i, t)$ is the probability density of a given instance of a set of molecules having the positions q_i and momenta p_i. The symplectic property of phase space implies that phase space is like an incompressible fluid, i.e. that the density is constant. Mathematically, this is expressed as

Poisson Bracket

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

$$\boxed{\begin{aligned} \frac{\partial \rho}{\partial t} &= -\{\rho, H\} \\ \frac{\partial \rho}{\partial t} &= -\sum_{i=1}^{3N}\left(\frac{\partial \rho}{\partial q_i}\frac{\partial H}{\partial p_i} - \frac{\partial \rho}{\partial p_i}\frac{\partial H}{\partial q_i}\right) \end{aligned}}$$

Liouville's Theorem
or
Liouville's Equation

change in prob density at a given point in phase space = − change in prob density as system moves in phase space.

This is a foundational equation for non-equilibrium stat mech. We will come back to it later. For now, just note that phase space has this important property.

Finally, note that Liouville's equation also applies at equilibrium.

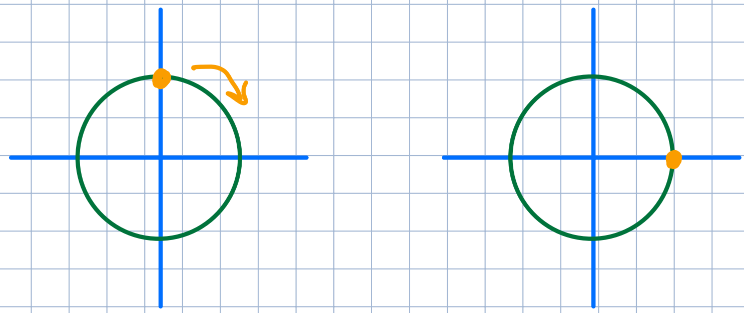
$$\frac{\partial \rho}{\partial t} = 0 \Rightarrow \{\rho, H\} = 0 \quad \text{and} \quad \rho = \rho_{eq}$$

D. Key concept 2: Symmetry

Above, we saw that dynamics can be thought of as motion in phase space. What does symmetry of this motion imply?

First, what do we mean by symmetry? We mean that when we do some kind of transformation, something doesn't change.

Example:



Rotation of a circle leaves the shape unchanged.

So, it is rotationally invariant or rotationally symmetric.

Invariance of the equations of motion to transformation are kinds of symmetries as well.

Noether's theorem says that if the system's dynamics have a symmetry, then this implies there is a conserved quantity that corresponds to that symmetry.

Example: time invariance.

Suppose that $H = H(q_i, p_i)$, not a function of time.

$$\frac{dH}{dt} = \frac{\partial H}{\partial t} + \{H, H\} \qquad \frac{\partial H}{\partial t} = 0 \text{ is implied from above}$$

$$\frac{dH}{dt} = \{H, H\} = \sum_{i=1}^{3N} \left(\frac{\partial H}{\partial q_i} \frac{\partial H}{\partial p_i} - \frac{\partial H}{\partial p_i} \frac{\partial H}{\partial q_i} \right) = 0$$

Time invariance implies that H doesn't change.

$\left(\frac{\partial H}{\partial t} = 0\right)$ $\qquad\qquad$ $\left(\frac{dH}{dt} = 0\right)$

In other words, energy is conserved if the equations of motion don't depend on time!

Other examples that I won't prove are that translational symmetry in phase space means that linear momentum is conserved and rotational symmetry in phase space means that angular momentum is conserved.

If the Hamiltonian doesn't explicitly depend on time, conserved quantities can be identified using the Poisson bracket

$$\frac{df}{dt} = \overbrace{\cancel{\frac{\partial f}{\partial t}}}^{0 \text{ if } f \neq f(t)} + \{f, H\}$$

therefore if $\{f, H\} = 0$ $\quad \frac{df}{dt} = 0$.

f is a constant of motion or f is "conserved."

Example : Linear momentum is conserved

$$\{p_j, H\} = \sum_{i=1}^{3N} \left[\frac{\partial p_j}{\partial q_i}\frac{\partial H}{\partial p_i} - \frac{\partial p_j}{\partial p_i}\frac{\partial H}{\partial q_i} \right] = -\frac{\partial H}{\partial q_j} = -\frac{\partial V}{\partial q_j}$$

zero b/c p & q are independent variables

$\delta_{ij} = 0$ for all $i \neq j$. 1 for $i = j$

$H = T(p) + V(q)$

if $V \neq V(q_j)$ then $\frac{\partial V}{\partial q_j} = 0$

translational invariance in q_j

Example : N-component harmonic oscillator

spring potential : $U = \sum_i \frac{1}{2} k x_i^2$ — spring constant

kinetic energy : $K = \sum_i \frac{1}{2} m v_i^2$ — particle mass

initial conditions :

$$x_i(0) = x_{i,0} \qquad v_i(0) = v_{i,0}$$

Compare and contrast with Lagrangian formalism.

$$L = K - U \qquad q_i = x_i \qquad \dot{q}_i = v_i$$

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}_i}\right) - \frac{\partial L}{\partial q_i} = 0 \Rightarrow \frac{d}{dt}\left(\frac{\partial L}{\partial v_i}\right) - \frac{\partial L}{\partial x_i} = 0$$

$$L = \sum_i \left[\frac{1}{2} m v_i^2 - \frac{1}{2} k x_i^2\right] \qquad \frac{\partial L}{\partial v_i} = m v_i \qquad \frac{\partial L}{\partial x_i} = k x_i$$

$$\frac{d}{dt}\left(m v_i\right) - k x_i = 0 \Rightarrow m \frac{dv_i}{dt} - k x_i = 0 \Rightarrow \frac{dv_i}{dt} - \frac{k}{m} x_i = 0$$

$$\boxed{\begin{array}{l} \dfrac{dv_i}{dt} - \omega^2 x_i = 0, \quad \omega^2 = k/m \\ v_i(0) = v_{i,0} \quad x_i(0) = x_{i,0} \end{array}}$$

Hamiltonian formalism

$$H = K + U \qquad q_i = x_i \qquad p_i = \frac{\partial L}{\partial \dot{q}_i} = \frac{\partial L}{\partial v_i} = m v_i \Rightarrow v_i = p_i/m$$

$$\dot{q}_i = \frac{\partial H}{\partial p_i} \qquad \dot{p}_i = -\frac{\partial H}{\partial q_i}$$ Hamilton's equations

$$\frac{dx_i}{dt} = \frac{\partial H}{\partial p_i} \qquad \frac{dp_i}{dt} = -\frac{\partial H}{\partial x_i}$$

$$H = \sum_i \left[\frac{1}{2} m v_i^2 + \frac{1}{2} k x_i^2\right] = \sum_i \left[\frac{p_i^2}{2m} + \frac{1}{2} k x_i^2\right]$$

$$\frac{\partial H}{\partial p_i} = \frac{p_i}{m} \qquad \frac{\partial H}{\partial x_i} = k x_i$$

$$\boxed{\begin{array}{ll} \dfrac{dx_i}{dt} = \dfrac{p_i}{m} & \dfrac{dp_i}{dt} = -k x_i \\ x_i(0) = x_{i,0} & p_i(0) = m v_i(0) \end{array}}$$

What if we add friction (a damped oscillator)? We don't get Hamilton's equations, because the system is not conservative.

The equations of motion are:

$$\frac{dx_i}{dt} = \frac{p_i}{m}, \qquad \frac{dp_i}{dt} = -k x_i - \gamma p_i$$

$$x_i(0) = x_{i,0}, \quad p_i(0) = m v_i(0)$$

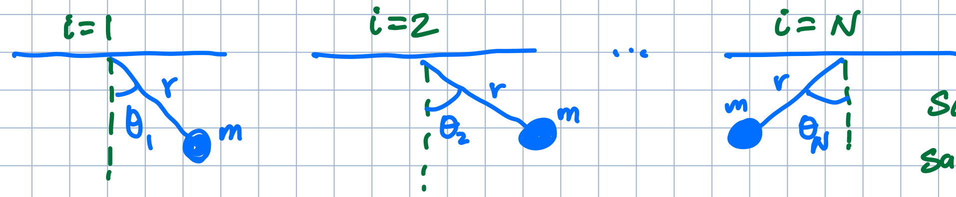
friction proportional to p_i with friction coefficient γ.

γ has units of $\frac{1}{\text{time}}$.

E. Appendix: Extra Examples

Example : N-component pendulum using Hamiltonian mechanics

Compare and contrast with the Lagrangian framework above.



same mass, m
same length, r

$$\left.\begin{aligned} K &= \sum_i \tfrac{1}{2} m r^2 \dot{\theta}_i^2 \\ U &= \sum_i \tfrac{1}{2} m g (r - r\cos\theta_i) \end{aligned}\right\} \quad H = K + U = \sum_i \left[\tfrac{1}{2} m r^2 \dot{\theta}_i^2 + \tfrac{1}{2} m g (r - r\cos\theta_i)\right]$$

Need to write in terms of generalized momenta

$$p_i = \frac{\partial L}{\partial \dot{q}_i} = \frac{\partial L}{\partial \dot{\theta}_i} = \frac{\partial K}{\partial \dot{\theta}_i} = m r^2 \dot{\theta}_i \Rightarrow \dot{\theta}_i = \frac{p_i}{m r^2}$$

$$H = \sum_i \left[\frac{1}{2} \frac{p_i^2}{m r^2} + \frac{1}{2} m g (r - r\cos\theta_i)\right]$$ find H in terms of p_i

Now get the equations of motion

$$\frac{dq_i}{dt} = \frac{\partial H}{\partial p_i}, \quad \frac{dp_i}{dt} = -\frac{\partial H}{\partial q_i} \Rightarrow \frac{d\theta_i}{dt} = \frac{\partial H}{\partial p_i} \quad \frac{dp_i}{dt} = -\frac{\partial H}{\partial \theta_i}$$

convert to θ_i, p_i

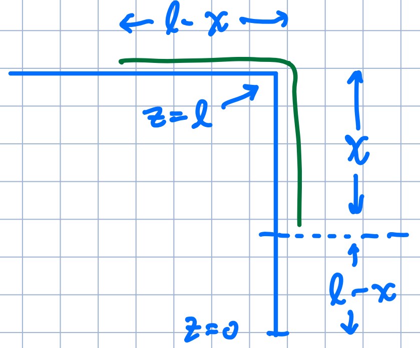
we need these derivatives

$$\frac{\partial H}{\partial p_i} = \frac{p_i}{m r^2} \qquad \frac{\partial H}{\partial \theta_i} = \frac{1}{2} m g r \sin\theta$$

now substitute back into Hamilton's Eq's.

$$\boxed{\begin{aligned} &\frac{d\theta_i}{dt} = \frac{p_i}{m r^2} \qquad \frac{dp_i}{dt} = -\frac{1}{2} m g r \sin\theta \\ &\theta_i(0) = \theta_{i,0} \qquad p_i(0) = m r^2 \dot{\theta}_{i,0} \end{aligned}}$$

Example: Chain sliding off a table



chain length: ℓ
chain mass: m
$\Big\}$ mass density $\lambda = \frac{m}{\ell}$

kinetic energy: $K = \frac{1}{2}\lambda \ell v^2$

$= \frac{1}{2} m v^2$

Potential energy: $U = \int F\, dz$

$= \int mg\, dz$

more potential energy:

- need a function for $m(z)$:

$m = 0$ when $z = \ell - x$
$m = \lambda x$ when $z = \ell$

slope $= \lambda$

$m = \lambda z + \text{const}$ ← solve for const

$0 = \lambda(\ell - x) + \text{const}$

$\text{const} = \lambda(x - \ell)$

$m(z) = \lambda(z + x - \ell)$

- Now integrate to find U:

$$U = \int_{\ell-x}^{\ell} m(z)\, g\, dz$$

$$= \int_{\ell-x}^{\ell} \lambda g(z + x - \ell)\, dz = \int_{\ell-x}^{\ell} \lambda g z\, dz + \int_{\ell-x}^{\ell} \lambda g(x-\ell)\, dz$$

$$= \left[\frac{\lambda g z^2}{2} + \lambda g(x-\ell) z\right]_{\ell-x}^{\ell} = \frac{1}{2}\lambda g \ell^2 + \lambda g(x-\ell)\ell - \frac{1}{2}\lambda g(\ell - x)^2 + \lambda g(\ell - x)^2$$

$$= -\frac{1}{2}\lambda g \ell^2 + \lambda g \ell x + \frac{1}{2}\lambda g(\ell - x)^2$$

$$= \cancel{-\frac{1}{2}\lambda g \ell^2} + \cancel{\lambda g \ell x} + \frac{1}{2}\lambda g(\cancel{\ell^2} - \cancel{2\ell x} + x^2)$$

$$= \frac{1}{2}\lambda g x^2$$

so, $K = \frac{1}{2}\lambda l v^2$ ∴ $U = \frac{1}{2}\lambda g x^2$

$L = K - U$, $\frac{\partial L}{\partial v} = \frac{\partial K}{\partial v} = \lambda l v$, $\frac{\partial L}{\partial x} = \frac{\partial U}{\partial x} = \lambda g x$

$\frac{d}{dt}\left(\frac{\partial L}{\partial v}\right) - \frac{\partial L}{\partial x} = 0 \Rightarrow \frac{d}{dt}(\lambda l v) - \lambda g x = 0$

$$\frac{dv}{dt} = \frac{g}{l} x$$

$$\boxed{\frac{d^2 x}{dt^2} = \frac{g}{l} x}$$