Lecture 11 – Lagrangian Mechanics

A. Newtonian Mechanics of Interacting Particles

We have talked about the statistics part of statistical mechanics, now we need a quick review of the mechanics part.

Aside: why the multiple names: statistical mechanics or statistical thermodynamics? they are equivalent. The former emphasizes the connection to physics.

The mechanics that you learned in introductory physics is Newtonian mechanics. For a set of N particles, Newton's Second Law is:

$$m_i \frac{d^2 \underline{r}_i}{dt^2} = \underline{F}_i$$

$\underline{r}_i$: position vector of particle i

$\underline{F}_i$: force on particle i

m_i : mass of particle i

Often, the force on a particle can be described by a potential, U. They are related by

$$\underline{F}_i = -\frac{\partial U}{\partial \underline{r}_i} = -\underline{\nabla}_i U \qquad U = U(\underline{r}_1, \underline{r}_2, \ldots, \underline{r}_N)$$

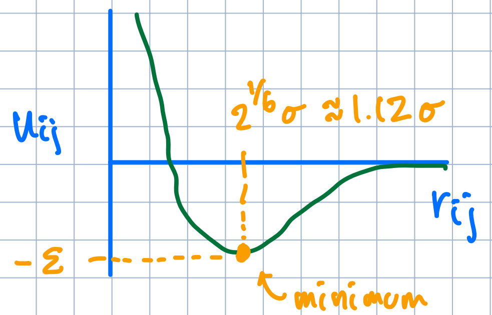
If there are no external forces, and only interactions between particles, then the total potential U can be simplified to a sum of pairwise potentials between the particles.

$$U = \sum_{i<j} u_{ij}(|\underline{r}_i - \underline{r}_j|)$$

$u_{ij}(r_{ij})$: pairwise potential

$r_{ij} = |\underline{r}_i - \underline{r}_j|$

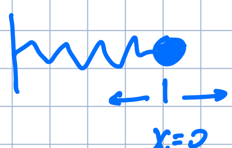
Example: Lennard Jones Potential



$$u_{ij}(r_{ij}) = 4\varepsilon\left[\left(\frac{\sigma}{r_{ij}}\right)^{12} - \left(\frac{\sigma}{r_{ij}}\right)^{6}\right]$$

We are going to need to compare Newtonian mechanics to two other types of mechanics (Lagrangian and Hamiltonian), so I want to do a simple example. We will also want a solved problem to discuss the concept of phase space.

Example: Harmonic Oscillator



Spring potential : $U = \frac{1}{2}kx^2$

particle mass : m

initial conditions: $x(0) = x_0$, $v(0) = v_0$

Newton's equation of motion:

$$m\frac{d^2x}{dt^2} = F \qquad F = -\frac{\partial u}{\partial x} = -\frac{\partial}{\partial x}\left(\frac{1}{2}kx^2\right) = -kx$$

$$m\frac{d^2x}{dt^2} = -kx \Rightarrow \frac{d^2x}{dt^2} + \frac{k}{m}x = 0 \qquad \text{let } \omega = \sqrt{\frac{k}{m}}$$

$$\frac{d^2x}{dt^2} + \omega^2 x = 0$$

ω is a frequency

$$[=]\sqrt{\frac{kg}{s^2}\cdot\frac{1}{kg}}$$

$$[=]\sqrt{1/s^2} = 1/s$$

This is a second order, homogeneous ODE. ω^2 is always positive, so solutions are given by:

$$x(t) = A\sin(\omega t) + B\cos(\omega t)$$, A & B are constants

Solving for A and B from the initial condition,

$$x(0) = A\sin(0) + B\cos(0) = B = x_0$$

$$v(t) = \frac{dx}{dt} = A\omega\cos(\omega t) - B\omega\sin(\omega t)$$

$$v(0) = A\omega\cos(0) - B\omega\sin(0) = A\omega = v_0, \quad A = \frac{v_0}{\omega}$$

So, the final solution is

$$\boxed{\begin{aligned} x(t) &= \frac{v_0}{\omega}\sin(\omega t) + x_0\cos(\omega t) \\ v(t) &= v_0\cos(\omega t) - x_0\omega\sin(\omega t) \end{aligned}}$$

B. Lagrangian Mechanics

Lagrange thought of mechanics differently than Newton. Rather than thinking of forces and inertia, he thought that Nature in some ways always acted optimally. So, in this way of thinking, the equations that govern dynamics minimize something. This something is called the action.

$$\underbrace{S}_{\text{action}} = \int_{t_1}^{t_2} \underbrace{L(\underline{q}_i, \dot{\underline{q}}_i, t)}_{\text{Lagrangian}^*}$$

$\underline{q}_i$: generalized coordinates

$\dot{\underline{q}}_i$: generalized velocities

N particles

* shorthand for: $L(\underline{q}_1, \underline{q}_2, \ldots, \underline{q}_N, \dot{\underline{q}}_1, \dot{\underline{q}}_2, \ldots, \dot{\underline{q}}_N, t)$

The generalized coordinates can be x, y, z, or they can be a coordinate transformation like r, θ, ϕ in spherical coordinates. The generalized velocities are time derivatives of the generalized coordinates. Mathematically, this is represented as

$$\begin{aligned} \underline{r}_1 &= \underline{r}_1(\underline{q}_1, \underline{q}_2, \ldots, \underline{q}_N) \\ \underline{r}_2 &= \underline{r}_2(\underline{q}_1, \underline{q}_2, \ldots, \underline{q}_N) \\ &\vdots \end{aligned} \quad \text{or} \quad \begin{aligned} \underline{q}_1 &= \underline{q}_1(\underline{r}_1, \underline{r}_2, \ldots, \underline{r}_N) \\ \underline{q}_2 &= \underline{q}_2(\underline{r}_1, \underline{r}_2, \ldots, \underline{r}_N) \\ &\vdots \end{aligned}$$

$$\underline{r}_N = \underline{r}_N(\underline{q}_1, \underline{q}_2, \cdots, \underline{q}_N) \qquad \underline{q}_N = \underline{q}_N(\underline{r}_1, \underline{r}_2, \ldots, \underline{r}_N)$$

The Lagrangian is like a "cost" that the particles pay. The action is a sum of the cost, and minimizing the action gives us the path or trajectory with the least cost.

Minimizing the action functional gives the Euler-Lagrange equations for the i^{th} particle

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{\underline{q}}_i}\right) - \frac{\partial L}{\partial \underline{q}_i} = 0 \qquad i = 1, 2, \ldots, N$$

The Lagrangian is given by

$$L = K(\dot{\underline{q}}_i) - U(\underline{q}_i)$$

K: kinetic energy

U: potential energy

So, the system "wants" to chart a path that balances kinetic energy and potential energy.

Let's show that the Euler-Lagrange equations give us the same thing as Newton's 2nd Law.

Equivalence of Lagrangian and Newtonian Mechanics:

Euler-Lagrange equation:

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

1 particle, constant m

$q = x$

$\dot{q} = \dot{x} = v$

Lagrangian:

$$L = K - U \qquad K = \frac{1}{2}mv^2$$

Put together:

doesn't depend on x

$$\frac{d}{dt}\left[\frac{\partial}{\partial v}\left(\frac{1}{2}mv^2\right)\right] - \frac{\partial}{\partial x}\left(\frac{1}{2}mv^2 - U\right) = 0$$

$$\frac{d}{dt}\left[mv\right] + \frac{\partial U}{\partial x} = 0 \Rightarrow m\frac{dv}{dt} = -\frac{\partial U}{\partial x} \Rightarrow \boxed{ma = F}$$

So, the Lagrangian way of doing mechanics is equivalent.

Why learn it?

- It can solve some problems much more easily.
  - problems with constraints
  - problems in different coordinates (no messy coordinate transforms)

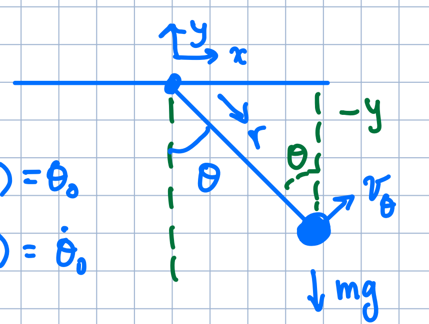
  The Euler-Lagrange Eq. is invariant to coordinate transforms (proof in book). This is the reason for "generalized coordinates."
- It comes up in stat thermo. "Story of your Life", Ted Chiang
- Additional physical principle / way of understanding the world.
- Connection to Hamiltonian mechanics (next)

To conclude, lets solve an example problem with it.

Example: Pendulum with a Lagrangian

$\theta(0) = \theta_0$

$\dot{\theta}(0) = \dot{\theta}_0$



What is our generalized coordinate?

r, θ? x, y? could be any.

θ is the easiest.

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{\theta}}\right) - \frac{\partial L}{\partial \theta} = 0 \qquad L = K - U$$

What is the kinetic energy?

$$K = \frac{1}{2}mv^2 \qquad v = r\cdot\dot{\theta} \Rightarrow K = \frac{1}{2}mr^2\dot{\theta}^2$$

What is the potential energy?

Assume $U=0$ at $y=-r$, the bottom of the pendulum.

$U = mg(y+r)$ $\quad y = -r\cos\theta \Rightarrow U = mg(r - r\cos\theta)$

Combine to get L:

$$L = K - U = \frac{1}{2} m r^2 \dot{\theta}^2 - mgr(1-\cos\theta)$$

$$\frac{\partial L}{\partial \dot{\theta}} = m r^2 \dot{\theta} \qquad \frac{\partial L}{\partial \theta} = -mgr\sin\theta$$

Plug into Euler-Lagrange Eq:

$$\frac{d}{dt}\left(m r^2 \dot{\theta}\right) + mgr\sin\theta = 0$$ m, g, r are constants

$$m r^2 \ddot{\theta} + mgr\sin\theta = 0 \Rightarrow \frac{d^2\theta}{dt^2} + \frac{g}{r}\sin\theta = 0$$

This is a nonlinear 2nd order ODE. We can solve it numerically or in the case where $\theta \ll 1$. In the latter case:

$$\sin\theta \simeq \theta + \frac{1}{2}\theta^2 + \ldots$$ Keep to 1st order only.

$$\frac{d^2\theta}{dt^2} + \frac{g}{r}\theta = 0 \qquad \theta(0) = \theta_0, \quad \dot{\theta}(0) = \dot{\theta}_0$$

same equation as harmonic motion, but $\omega^2 = g/r$.

$$\theta(t) = \frac{\dot{\theta}_0}{\omega}\sin(\omega t) + \theta_0\cos(\omega t)$$

$$\dot{\theta}(t) = \dot{\theta}_0\cos(\omega t) + \theta_0\omega\sin(\omega t)$$

$$\omega = \sqrt{g/r}$$

check units:

$\theta = \text{rad}$, $\dot{\theta} = \text{rad}/s$

$$\omega = \sqrt{\frac{cm/s^2}{cm}} = \sqrt{\frac{1}{s^2}} = \frac{1}{s} \checkmark$$

For the numerical solution:

$$\frac{d^2\theta}{dt^2} + \omega^2\sin\theta = 0, \quad \omega^2 = g/r \Rightarrow \frac{d\dot{\theta}}{dt} = -\omega^2\sin\theta, \quad \dot{\theta}(0) = \dot{\theta}_0$$

$$\frac{d\theta}{dt} = \dot{\theta}, \quad \theta(0) = \theta_0$$