Computing the Universe, Dynamics II: Hamiltonian dynamics

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1 Why bother getting fancy?

Why not just use Newton's Laws for everything? I gave a philosophical motivation in the first lecture. Today we will see that an alternative approach provides a qualitatively unique understanding that detailed solutions of coupled ODEs do not.

Recall, from your intermediate mechanics class, the *Principle of Virtual Work*. This says that the work done in any virtual displacement consistent with the constraints must be zero. For conservative systems, the potential energy, W, must be an extremum of the equilibrium and a minimum if stable. The beauty is that this principle can be stated without regard to number of bodies, choice of coordinates, and other complications arising in complex configurations.

2 Lagrangian mechanics

Can a similar principle be found to describe the solution to Newton's equations of motion? What function takes the place of the potential? The basic idea of Lagrange was to imagine a fictitious force equal to minus the rate of change of momentum for each particle. Each point of the trajectory may be considered, then, to be an equilibrium between real and fictitious forces. Applying the principle of virtual work to this notion produces the expression:

$$\sum_i (\mathbf{f}_i \cdot \delta\mathbf{x}_i - \dot{\mathbf{p}}_i \cdot \delta\mathbf{x}_i),$$

where I am using $\mathbf{p} = m\mathbf{v} = m\dot{\mathbf{x}}$ for consistency with general usage; previously I had been tacitly setting $m = 1$ so I didn't have to clutter up the notation. The δ quantities denote small (virtual) displacements and the sum over i indexed particle coordinates. Because the displacements are independent at different times, the integral of this sum must also vanish over some segment of the evolution:

$$\int_{t_1}^{t_2} dt \sum_i (\mathbf{f}_i - \dot{\mathbf{p}}_i) \cdot \delta\mathbf{x}_i = 0.$$

Integrating this expression by parts yields:

$$\int_{t_1}^{t_2} dt \left[-\delta W + \sum_i \mathbf{p}_i \frac{d}{dt}(\delta\mathbf{x}_i)) \right] - \sum_i \mathbf{p}_i \cdot \delta\mathbf{x}_i|_{t_1}^{t_2} = 0.$$

In order to be able to write down the integral, we are tacitly assuming that we know that the trajectory goes from some point $\mathbf{x}(t_1)$ to $\mathbf{x}(t_2)$ so the displacements must vanish at t_1 and t_2 and therefore the integrated term vanishes. Now, note that $\mathbf{p}_i d(\delta\mathbf{x}_i)/dt = \mathbf{p}_i \cdot \delta\mathbf{v} = \delta T_i$ where $T_i = m_i v_i^2/2 = p_i^2/2m_i$. Putting this all together, our integral becomes:

$$\int_{t_1}^{t_2} dt\,[-\delta W + \delta T] = \delta \int_{t_1}^{t_2} dt\,[T - W] = \int_{t_1}^{t_2} dt L = 0.$$

This is our new law of mechanics! It says that the desired solution is one that extremizes the integral of the function L. The function

L, as most of you know, is called the *Lagrangian*. Note that we haven't specified any coordinate system; the new law of mechanics is coordinate-free!

3 Hamilton's equations

Lagrangian mechanics has many uses but it also has some fundamental flaws. Fortunately, these have been fixed up by Hamilton and Jacobi, as I will now describe.

The problem is that the new equations of motion follow from the variation of $L = L(\mathbf{q}, \dot{\mathbf{q}}, t)$ where $\mathbf{q}$ is a vector of coordinates. The fact that L depends on both a set of coordinates and its time derivatives makes it difficult to choose a general coordinate system. For example, a velocity dependent coordinate system would depend on acceleration. Velocity dependent coordinates are natural in non-inertial systems, such as the local standard of rest of the Sun about the Galaxy whose coordinates depend on angular momentum.

Hamilton realized that there was no reason that momenta could not act as coordinates with an appropriate change of variables. This change of variables has the constraint that the extremization of L has to remain the same. Those of you that recall you thermodynamics will remember the *Legendre transformation* which accomplishes the same task. In short, adding a perfect differential to L is the same as adding a constant since the value of the differential is determined by its value at the end points. Explicitly, the total differential of L is:

$$dL = \mathbf{p} \cdot d\dot{\mathbf{q}} + \frac{\partial L}{\partial \mathbf{q}} \cdot d\mathbf{q} + \frac{\partial L}{\partial t} dt$$

and I have made the identification $\mathbf{p} = \frac{\partial L}{\partial \dot{\mathbf{q}}}$ which follows naturally in the Lagrangian method. Now, adding $-d(\mathbf{p} \cdot \dot{\mathbf{q}})$ to this expression yields

$$d(L - \mathbf{p}\cdot\dot{\mathbf{q}}) = -dH = -\dot{\mathbf{q}}\cdot d\mathbf{p} + \frac{\partial L}{\partial \mathbf{q}}\cdot d\mathbf{q} + \frac{\partial L}{\partial t}dt$$

and we have changed our variation in L to a new one $H = H(\mathbf{p},\mathbf{q})$. This new function H is called the Hamiltonian. Note the new variables! Returning to the variational principle, we may write it in terms of H using $L = \mathbf{p}\cdot\dot{\mathbf{q}}$:

$$\delta\int_{t_1}^{t_2} dtL = \int_{t_1}^{t_2} dt\,\delta\left(\mathbf{p}\cdot\dot{\mathbf{q}} - H(\mathbf{p},\mathbf{q})\right) = 0.$$

Now doing the variation in the new variables gives:

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

The total derivative does not effect the variation, as we have discussed. The variations in $\mathbf{p}$ and $\mathbf{q}$ are now independent. For example, there is no restriction that a change in $\delta\mathbf{p}$ correspond to a change $\mathbf{q}+\delta\mathbf{q}$ and $\mathbf{p}+\delta\mathbf{p}$. Therefore, to hold everywhere along the trajectory, the terms in parentheses must vanish everywhere and we are left with the following equations:

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

These are *Hamilton's equations*.

3.1 Coordinate choices: canonical transformations

As advertised, these equations do not depend on the choice of coordinates and take the same form regardless of the choice (consistent with the Lagrangian variation, of course). This is a major feature of Hamiltonian dynamics and simple to demonstrate. If two coordinates (both the positions and momenta) have the same *content*, then they must obey variational equations which take the same form:

$$\delta \int dt \, (\mathbf{p} \cdot \dot{\mathbf{q}} - H) = \delta \int dt \, \left(\mathbf{P} \cdot \dot{\mathbf{Q}} - \mathcal{H}\right)$$

This may seem like an odd distinction to make but is a consequence of not having make any assumptions about the coordinates to start. Rewriting this as

$$\delta \int dt \left[(\mathbf{p} \cdot \dot{\mathbf{q}} - H) - \left(\mathbf{P} \cdot \dot{\mathbf{Q}} - \mathcal{H}\right) \right] = 0$$

immediate shows that the term in square brackets must be identical along the trajectory up to some total differential:

$$(\mathbf{p} \cdot \dot{\mathbf{q}} - H) - \left(\mathbf{P} \cdot \dot{\mathbf{Q}} - \mathcal{H}\right) = \frac{dF}{dt}.$$

The function F must be well-behaved in the usual physicist's sense but otherwise is arbitrary. For convenience, people usually write: $F = S(\mathbf{P}, \mathbf{q}, t) - \mathbf{P} \cdot \mathbf{Q}$. Then, the expansion becomes

$$\begin{aligned} \mathbf{p} \cdot d\mathbf{q} - H dt &= \mathbf{P} \cdot d\mathbf{Q} - \mathcal{H} dt + d\,(S - \mathbf{P} \cdot \mathbf{Q}) \\ &= \frac{\partial S}{\partial \mathbf{q}} \cdot d\mathbf{q} + \left(\frac{\partial S}{\partial \mathbf{P}} - \mathbf{Q} \right) \cdot d\mathbf{P} - \mathcal{H} dt + \frac{\partial S}{\partial t} dt. \end{aligned}$$

Identifying coefficients, we then must demand that

$$\mathbf{p} = \frac{\partial S}{\partial \mathbf{q}}, \qquad \mathbf{Q} = \frac{\partial S}{\partial \mathbf{P}}, \qquad H = \mathcal{H} - \frac{\partial S}{\partial t}.$$

In other words, we have demonstrated that any transformation to new variables can be generated by choosing some function S. The function S has the dimensions of an action and is sometimes called an *action function* and this transformation is called a *canonical transformation*[1].

4 Jacobi's trick

Hamiltonian dynamics leads to many fundamental insights into the structure of dynamical systems. One of the most useful ones was based on the observation by Jacobi: if one can find the canonical transformation which makes the new Hamiltonian identically zero, $\mathcal{H} = 0$, then $\mathbf{P}$ and $\mathbf{Q}$ are integrals of the motion (conserved quantities) and the problem is solved for good!

Do do this we need:

$$\mathcal{H} = 0 = H + \frac{\partial S}{\partial t}.$$

Now, $H = H(\mathbf{p}, \mathbf{q}, t) = H(\partial S/\partial \mathbf{q}, \mathbf{q}, t)$ so the condition $\mathcal{H} = 0$ implies

$$H\left[\left(\frac{\partial S}{\partial \mathbf{q}}\right), \mathbf{q}, t\right] + \frac{\partial S}{\partial t} = 0$$

and this is called the *Hamilton-Jacobi* equation (H-J). As you might have guessed, we did not get anything for free here. Now we have to solve a new implicit partial differential equation for S. Once we solve for S, the desired coordinates follow from $\mathbf{Q} = \partial S/\partial \mathbf{P}$ and the n constants of integration from the PDE can be identified as the momentum coordinates $\mathbf{P}$.

One problem with this is that $\mathbf{P}$ and $\mathbf{Q}$ are constant but the transformation, through S, is now time dependent. Let's decide to stick a

[1] Other choices of the generating function F give different variables, see Goldstein for an enumeration of all 4 types possible.

time-independent S. Then, the H-J equation becomes

$$H\left[\frac{\partial S}{\partial \mathbf{q}}, \mathbf{q}\right] = \mathcal{H}(\mathbf{P}) \equiv E = \text{constant}.$$

The new Hamiltonian $\mathcal{H}$ is now a constant rather than zero. Because we have identified $\mathbf{P}$ with the constants of integration, $\mathcal{H}$ will now be some function of these constants. Hamilton's equation now give:

$$\begin{aligned} \dot{\mathbf{P}} &= -\frac{\partial \mathcal{H}}{\partial \mathbf{Q}} = 0 \\ \dot{\mathbf{Q}} &= -\frac{\partial \mathcal{H}}{\partial \mathbf{P}} = \text{constant} \end{aligned}$$

which has the trivial solution: $\mathbf{P} = \text{constant}$, $Q(t) = \partial\mathcal{H}/\partial\mathbf{P}t + \mathbf{Q}_o$! In other words Q increases linearly with time. This fact may be exploited to choose variables that are phases (angle-like) just as in the harmonic oscillator; such motion is called *multiply periodic*.

5 Actions

How do we choose such multiply periodic variables? We want:

$$2\pi = \oint d\mathbf{q} = \oint d\mathbf{q} \cdot \frac{\partial Q}{\partial \mathbf{q}}.$$

For some coordinate Q. Now use the fact that $Q = \partial S/\partial P|_{\mathbf{q}}$ in the above to get

$$2\pi = \oint d\mathbf{q} \cdot \frac{\partial^2 S}{\partial \mathbf{q} \partial P} = \frac{\partial}{\partial P} \oint d\mathbf{q} \cdot \mathbf{p}.$$

This is satisfied if we take:

$$P = \frac{1}{2\pi} \oint d\mathbf{q} \cdot \mathbf{p} = \frac{1}{2\pi} \{\text{phase space area}\}.$$

This new variable is usually called *the action* and usually denoted by I or J.

Next lecture will further explore the implications of this solution to the H-J equation. It is fundamental for understanding orbits and their classification, the long-term evolution of galaxies, the construction of galactic models, just to name a few applications.