Oct. 28

Hamiltonian Mechanics

To continue our study of nonlinear mechanical systems, we need more formalism. What we need, in particular, is a much more effective way to visualize the solutions of classical mechanical equations as flows. We would like to use this as a tool for analyzing nonlinear interactions. This tool is provided by the Hamiltonian approach to mechanics.

So far in this course, our discussion has been based on the coordinate variables q_i, which obey second-order differential equations. However, as we saw even in the first lecture, it is much easier to visualize the solution to a set of equations when they are written in first-order form. The motion is then, in a very straightforward way, a flow in the appropriate space. Hamiltonian mechanics recasts a general Lagrangian system as a flow of this type, and one, moreover, with special simplifying properties.

We can begin from our general formulation of Lagrangian mechanics in terms of generalized coordinates. These coordinate variables obey the Euler-Lagrange equations

$$\frac{d}{dt} p_i = \frac{\partial L}{\partial q_i}$$

where

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

are the *conjugate momenta* to the coordinates q_i. In the normal situation in which L is at most second order in time derivatives, the p_i are first order in the $\dot{q}_i$, with additional dependence on the q_i without derivatives. It is suggestive, then, that we can find a system of first-order equations by eliminating $\dot{q}_i$ in terms of the p_i and writing equations for the q_i and p_i.

This change of the variables is accomplished by a *Legendre transformation.* You might recall from thermodynamics that we can transform from one set of variables to another by a manipulation on the basic thermodynamic function. For example, we often begin the construction of thermodyanics from the basic relationship of the energy and the entropy

$$S(E) \quad \text{or} \quad E(S)$$

Temperature is defined as

$$\frac{1}{T} = \frac{dS}{dE} \quad \text{or} \quad T = \frac{dE}{dS}$$

It is more useful, however, to consider temperature as the basic variable that is fixed in a physical situation. To convert from a system based on entropy to a system based on temperature, we define a new thermodyamics function, the *free energy*, by

$$F = E - TS$$

The free energy has the property that it is free of explicit dependence on S. If we compute the derivative of F with respect to T, we find

$$\frac{dF}{dT} = \frac{dS}{dT}\Big[\underbrace{\frac{dE}{dS} - T}_{=0}\Big] - S = -S$$

If we know the relation between S and T, we can now recast F complete as a function of T.

In mechanics, we could also search for an appropriate Legendre transformation to assist us in converting from the set of variables $\{q_i, \dot{q}_i\}$ to the variables $\{q_i, p_i\}$. However, we already have the appropriate object at hand. The quantity

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

is the conserved energy in the case that L has no explicit dependence on t. The quantity H is called the *Hamiltonian.* The derivative of the Hamiltonian with respect to p_i with all q_i fixed is given by

$$\left.\frac{\partial H}{\partial p_i}\right|_q = \left.\frac{\partial \dot{q}_j}{\partial p_i}\right|_q \Big[\underbrace{-\frac{\partial L}{\partial \dot{q}_j} + p_j}_{0}\Big] + \dot{q}_i = \dot{q}_i$$

so, in exactly the same way, H can be thought of as a function of the q_i and p_i. The $\dot{q}_i$ can be written as a function of these variables by solving the equations

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

At the same time, we can compute the derivative of H with respect to the q_i with all p_i held fixed. This gives

$$\left.\frac{\partial H}{\partial q_i}\right|_p = \left.\frac{\partial \dot{q}_j}{\partial q}\right|_p \Big[\underbrace{-\frac{\partial L}{\partial \dot{q}_j} + p_j}_{0}\Big] - \frac{\partial L}{\partial q_i} = -\frac{\partial L}{\partial q_i}$$

The final answer is the right-hand side of the Euler-Lagrange equation, now written as a function of q_i and p_i. Then the first time derivatives of q_i and p_i are given by the equations

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

where H is a function of the q_i and p_i. These are the *Hamiltonian equations of motion.* We have now converted our Lagrangian system with n variables to a system of $2n$ first-order equations that corresponds to a flow through the space they define. This $2n$ dimensional space is called *phase space.*

It is useful to work out a few simple examples. Consider first a particle moving in 1 dimension in a potential $V(x)$. The Lagrangian is

$$L = \frac{1}{2} m \dot{x}^2 - V(x)$$

For this system,

$$p = m\dot{x}$$

so it is easy to convert between $\dot{x}$ and p. The Hamiltonian is

$$H = p\dot{x} - L = p\dot{x} - \frac{1}{2} m \dot{x}^2 + V(x)$$

or

$$H = \frac{p^2}{2m} + V(x)$$

The Hamiltonian equations are

$$\dot{x} = \frac{p}{m} \qquad \dot{p} = -\frac{dV}{dx}$$

and these give a flow in a 2 dimensional phase space.

Consider next the motion of a particle in a plane, in polar coordinates. The Lagrangian is

$$L = \frac{1}{2} m \left[\dot{r}^2 + r^2 \dot{\phi}^2 \right] - V(\vec{r})$$

The conjugate momenta are

$$p_r = m\dot{r} \qquad\qquad p_\phi = m r^2 \dot{\phi}$$

Then we can easily see that the Hamiltonian is

$$H = \frac{1}{2} \frac{p_r^2}{m} + \frac{1}{2} \frac{p_\phi^2}{m r^2} + V$$

In this case, H has a more complicated dependence on the coordinate r. However, for the case in which V is rotationally symmetric, the equations of motion for ϕ and p_ϕ are very simple

$$\dot{\phi} = \frac{p_r}{m r^2} \qquad\qquad \dot{p}_\phi = 0$$

The constancy of p_ϕ is the expression of Noether's theorem in Hamiltonian formalism.

A more involved example is given by the motion of a particle in a background electromagnetic field. We saw that this system is described by the Lagrangian

$$L = \frac{1}{2} m (\dot{\vec{x}})^2 + \frac{q}{c} \vec{A} \cdot \dot{\vec{x}} - q\phi$$

where $\phi(\vec{x},t)$ and $\vec{A}(\vec{x},t)$ are evaluated at the position of the particle at time t. The conjugate momentum to $\vec{x}$ is

$$\vec{p} = m\dot{\vec{x}} + \frac{q}{c}\vec{A}$$

Thus, to form the Hamiltonian, we must eliminate $\dot{\vec{x}}$ using the relation

$$\dot{\vec{x}} = \frac{1}{m}\left(\vec{p} - \frac{q}{c}\vec{A}\right)$$

Then

$$\mathcal{H} = \vec{p}\cdot\frac{\left(\vec{p} - \frac{q}{c}\vec{A}\right)}{m} - \frac{1}{2}\frac{\left(\vec{p} - \frac{q}{c}\vec{A}\right)^2}{m} - \frac{q}{c}\vec{A}\cdot\frac{\left(\vec{p} - \frac{q}{c}\vec{A}\right)}{m} + q\phi$$

that is

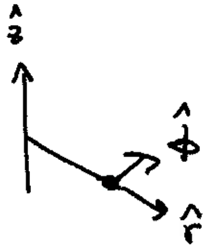
$$\mathcal{H} = \frac{1}{2}\frac{\left(\vec{p} - \frac{q}{c}\vec{A}\right)^2}{m} + q\phi$$

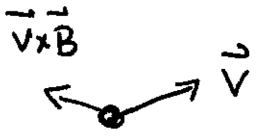
The equation of motion for $\vec{p}$ is

$$\dot{\vec{p}} = -\frac{\partial H}{\partial \vec{x}} = -q\vec{\nabla}\phi + \frac{q}{c}\vec{\nabla}A^j \cdot \frac{\left(p - \frac{q}{c}A\right)^j}{m}$$

This is not quite in the form of the Lorentz force equation, but it becomes the Lorentz force equation when we convert $\vec{p}$ back to $\dot{\vec{x}}$.

The special relevance of $\vec{p}$ is clearer in particular situations. Consider, for example, a particle executing a circular orbit in a constant magnetic field. Let the $\vec{B}$ field be in the $-\hat{z}$ direction:





The Lagrangian and Hamiltonian formalism uses the $\vec{A}$ field. An $\vec{A}$ that generates this $\vec{B}$ is

$$\vec{A} = -\frac{1}{2}\vec{r}\times\vec{B} \quad \text{or} \quad A^j = -\frac{1}{2}\epsilon^{jkl}x^k B^l$$

For this orientation of the $\vec{B}$ field,

$$\vec{A} = -\frac{1}{2} r B \hat{\phi}$$

and we might as well take the origin of $\vec{r}$ at the center of the circle. The velocity of the particle is

$$\dot{\vec{x}} = v\hat{\phi}$$

Then

$$\vec{p} = \left(mv - \frac{1}{2}\frac{qB}{c}r\right)\hat{\phi} = \left(m\omega - \frac{1}{2}\frac{qB}{c}\right) r\hat{\phi}$$

where $\omega = v/r$. The Hamiltonian equation of motion is

$$(\dot{\vec{p}})^i = \frac{q}{c}\left(-\frac{1}{2}\epsilon^{jil}B^l\right)\dot{x}^j$$

or

$$\dot{p}^i = -\frac{qv}{2c}\,\epsilon^{\hat{\phi} i \hat{z}}(-B)$$

$$\epsilon^{\hat{\phi} i \hat{z}} = +\,\epsilon^{\hat{z}\hat{\phi} i} = (\hat{z}\times\hat{\phi})^i$$

so that

$$\dot{\vec{p}} = -\hat{r}\,\frac{qB}{2c}\cdot\omega r$$

All of this is consistent only if

$$p = \frac{qB}{2c}\,r \qquad \underline{\text{and}} \qquad mv = p + \frac{1}{2}\frac{qBr}{c} = \frac{qBr}{c}$$

So we find that

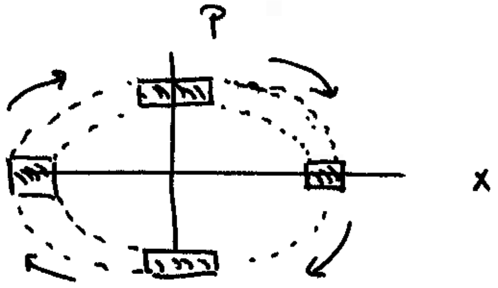
$$\omega = \frac{qB}{mc}$$

the familiar *cyclotron frequency*, and

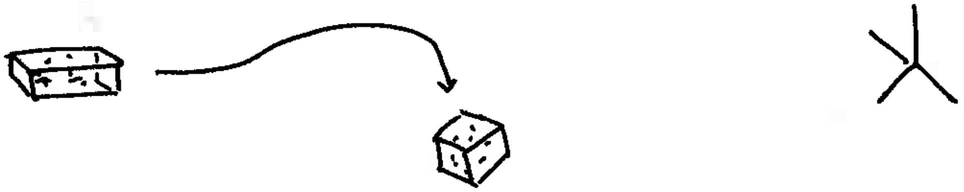
$$\vec{p} = \frac{m\omega r}{2}\,\hat{\phi} \qquad \frac{q\vec{A}}{c} = -\frac{m\omega r}{2}\,\hat{\phi} \qquad \vec{v} = \omega r\,\hat{\phi}$$

With these examples in hand, I will return to the formal aspects of Hamiltonian mechanics. Now that we have written a general Lagrangian system as a flow in phase space, what kind of flow is this? What special properties does this flow have?

Hamiltonian flows have one property that is very famous and is used for many applications in physics: Hamiltonian flows preserve volume in phase space. That is, if we choose a small box in phase space and compute the position of this box at a later time by moving the position of the box according to the Hamiltonian equations, the volume of the box will remain unchanged. In a 2 dimensional phase space, then, Hamiltonian evolution carries



In a higher dimensional phase space, similarly,



The shape of the original region may be distorted, but its phase space volume is preserved. This result is called *Liouville's theorem.*

To prove Liouville's theorem, we need only consider the change in a small volume. Choose a point

$$q_1 \text{ --- } q_n \quad p_1 \text{ --- } p_n$$

and consider the infinitesimal phase space volume element at this point

$$dq_1 \cdots dq_n \, dp_1 \cdots dp_n$$

After a time Δt, each coordinate and momentum has evolved according to

$$q_i \to q_i + \dot{q}_i \, \Delta t = q_i + \frac{\partial H}{\partial p_i} \Delta t$$
$$p_i \to p_i + \dot{p}_i \, \Delta t = p_i - \frac{\partial H}{\partial q_i} \Delta t$$

For finite t, we obtain the new location by integrating these differential equations. Call the new coordinates

$$q_1' \cdots q_n' \quad p_1' - - p_n'$$

The change of variables from the old coordinates to the new ones has the Jacobian

$$\mathcal{J}(t) = \frac{\partial(q_1' \cdots q_n' \, p_1' \cdots p_n')}{\partial(q_1 - q_n \, p_1 \cdots p_n)}$$

Liouville's theorem follows if the determinant of this Jacobian matrix is equal to 1.

It is illustrative to compute this determinant first for a 2 dimensional phase space, that is, for a system described by one q and one p. In that case, for a small time interval Δt,

$$\mathcal{J} = \frac{\partial(q' p')}{\partial(q p)} = \begin{pmatrix} 1 + \frac{\partial^2 H}{\partial p \partial q} \Delta t & \frac{\partial^2 H}{\partial p^2} \Delta t \\ - \frac{\partial^2 H}{\partial q^2} \Delta t & 1 - \frac{\partial^2 H}{\partial q \partial p} \Delta t \end{pmatrix}$$

The determinant of this matrix is

$$\det \mathcal{J} = 1 + \frac{\partial^2 H}{\partial p \partial q} \Delta t - \frac{\partial^2 H}{\partial q \partial p} \Delta t + \mathcal{O}((\Delta t)^2)$$
$$= 1 + \mathcal{O}((\Delta t)^2)$$

Thus

$$\frac{d}{dt}\det \mathcal{J}(t) = 0$$

and so, since

$$\det \mathcal{J}(t) = 1 \qquad \text{for} \quad t=0$$

the determinant must be equal to 1 for all times.

The argument is not much harder for systems with many degrees of freedom. The Jacobian is a $2n \times 2n$ matrix with the block structure

$$\mathcal{J}_{ij} = \left(\begin{array}{c|c} \dfrac{\partial q_i'}{\partial q_j} & \dfrac{\partial q_i'}{\partial p_j} \\ \hline \dfrac{\partial p_i'}{\partial q_j} & \dfrac{\partial p_i'}{\partial p_j} \end{array} \right)$$

For a small time interval Δt, this reads

$$\mathcal{J} = \left(\begin{array}{c|c} \delta_{ij} + \dfrac{\partial^2 H}{\partial p_i \partial q_j} \Delta t & \dfrac{\partial^2 H}{\partial p_i \partial p_j} \Delta t \\ \hline - \dfrac{\partial^2 H}{\partial q_i \partial q_j} \Delta t & \delta_{ij} - \dfrac{\partial^2 H}{\partial q_i \partial p_j} \Delta t \end{array} \right) + \mathcal{O}((\Delta t)^2)$$

This matrix is very close to 1; write it as

$$\mathcal{J} = 1 + \Delta + \mathcal{O}(\Delta^2)$$

We can compute its determinant from the general formula for the determinant of a matrix close to 1,

$$\det(1+\Delta+\cdots) = 1 + \operatorname{tr}\Delta + \cdots$$

Here is a proof of this formula: Diagonalize Δ, and call the eigenvalues d_i. Then

$$\det(1+\Delta) = \prod_i (1+d_i) = 1 + \sum_i d_i + \cdots$$

$$= 1 + \operatorname{tr}\Delta + \cdots$$

Applying this result to the Jacobian determinant in the form above, we find

$$\det \mathcal{J} = 1 + \operatorname{tr}\left(\begin{array}{c|c} \frac{\partial^2 H}{\partial p_i \partial q_j} & \frac{\partial^2 H}{\partial p_i \partial p_j} \\ \hline -\frac{\partial^2 H}{\partial q_i \partial q_j} & -\frac{\partial^2 H}{\partial q_i \partial p_j} \end{array}\right)\Delta t$$

$$= 1 + \Big(\underbrace{\sum_i \frac{\partial^2 H}{\partial p_i \partial q_i} - \sum_i \frac{\partial^2 H}{\partial q_i \partial p_i}}_{0\ !}\Big)\Delta t + O((\Delta t)^2)$$

Then, in general

$$\frac{d}{dt}\det \mathcal{J}(t) = 0$$

and so the Jacobian equals 1 for all times. Notice that this result follows for any system for which the equations of motion are of the Hamiltonian form. If the Hamiltonian depends explicitly on time, energy will not be conserved, but still Liouville's theorem will be valid.

In fact, the Jacobian above seems to have more even structure than is captured by Liouville's theorem. To understand this structure, I will write the Hamiltonian equations in a matrix form. To do this, introduce the antisymmetric $2n \times 2n$ dimensional matrix E,

$$E = \left(\begin{array}{c|c} 0 & \underline{1} \\ \hline -\underline{1} & 0 \end{array} \right)$$

We encountered this object earlier in our discussion of the Lie groups $Sp(2n)$. The matrix E appears naturally in the Hamiltonian formalism. Let

$$\underline{x} = \begin{pmatrix} q_1 \\ \vdots \\ q_n \\ p_1 \\ \vdots \\ p_n \end{pmatrix}$$

Then the Hamiltonian equations of motion take the form

$$\dot{x}_i = E_{ij} \frac{\partial H}{\partial x_j}$$

Now consider a change of variables

$$x_i \to y_i(x)$$

We might ask, under what conditions are the equations of motion of the y_i also a Hamiltonian flow? Explicitly, $\dot{y}_i$ is given by

$$\dot{y}_i = \frac{\partial y_i}{\partial x_j} \dot{x}_j = \frac{\partial y_i}{\partial x_j} E_{jk} \frac{\partial y_l}{\partial x_k} \frac{\partial H}{\partial y_l}$$

The matrix

$$\partial_{ij} = \frac{\partial y_i}{\partial x_j}$$

is the Jacobian of the transformation from the x_i to the y_i. Then we have

$$\dot{y} = \mathcal{J} \cdot E \cdot \mathcal{J}^T \cdot \frac{\partial H}{\partial y}$$

This is of the Hamiltonian form if

$$\mathcal{J} E \mathcal{J}^T = E$$

As we saw earlier in the course, this is exactly the condition that the linear transformation

$$\xi \to \mathcal{J}^T \xi$$

preserves the antisymmetric inner product

$$\eta_i E_{ij} \xi_j$$

The transformations of this type that belong to $SU(2n)$ form the compact Lie group $Sp(2n)$. In this context, $\mathcal{J}$ is a matrix with real entries and the corresponding symplectic group is a noncompact group obtained from $Sp(2n)$ by analytic continuation. Nevertheless, the basic algebraic characterization of the infinitesimal elements of this group remain the same. If we write $\mathcal{J}$ in infinitesimal form

$$\underline{\mathcal{J}} = 1 + \underline{K} \, \Delta\alpha$$

where α is a continuous parameter of the transformation, then the infinitesimal form of the relation

$$\mathcal{J} E \mathcal{J}^T = E$$

is

$$\mathcal{K} E + E K^T = 0$$

This implies the property $E^T = -E$

$$\mathcal{K} E = (KE)^T$$

We can check this result by showing that it is a property of the Jacobian associated with time evolution. We saw earlier that, for time evolution

$$\mathcal{J} = 1 + K \, \Delta t$$

where

$$\mathcal{K}_{ij} = \left(\begin{array}{c|c} \frac{\partial^2 H}{\partial p_i \partial q_j} & \frac{\partial^2 H}{\partial p_i \partial p_j} \\ \hline -\frac{\partial^2 H}{\partial q_i \partial q_j} & -\frac{\partial^2 H}{\partial q_i \partial p_j} \end{array} \right)$$

Then

$$\mathcal{K} E = \left(\begin{array}{c|c} -\frac{\partial^2 H}{\partial p_i \partial p_j} & \frac{\partial^2 H}{\partial p_i \partial q_j} \\ \hline \frac{\partial^2 H}{\partial q_i \partial p_j} & -\frac{\partial^2 H}{\partial q_i \partial q_j} \end{array} \right)$$

and this is indeed a symmetric matrix.

In Hamiltonian dynamics, a change of variables whose Jacobian is symplectic in this sense is called a *canonical transformation.* Such a transformation converts one Hamiltonian system into another. Time translation is a canonical transformation, but we can also design our own canonical transformations in such a way that they are useful for simplifying problems of mechanics. I will give some examples in the next lecture.