Hamiltonian Mechanics

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1 Brief Notes

For a mechanical system with no spatial derivatives (a system of particles) and for the Lagrangian $L = T - V$, Lagrange's equations are

$$\frac{\partial}{\partial t}\left(\frac{\partial L}{\partial \dot{q}_i}\right) - \frac{\partial L}{\partial q_i} = 0$$

where q_i are the generalized displacement degrees of freedom, T is the kinteic energy, and V is the potential. The conjugate momenta are defined as

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

which means that from Lagrange's equations, we have

$$\dot{p}_i = \frac{\partial L}{\partial q_i}$$

These are the necessary preliminary ideas we need to construct the Hamiltonian formulation of mechanics. Note that the given form of Lagrange's equations does not work for continuous elastic systems where spatial derivatives of the displacement variable arise. Spatial derivatives would enter Lagrange's equations in this case. This formulation restricts us to discretized elastic systems. The goal of Hamiltonian mechanics is to formulate a system of governing equations which are first order in time. In the Lagrangian version of mechanics, the state of the system is specified by the n displacement degrees of freedom. Velocities are computed by taking time derivatives of the displacement. But because the governing equations are second order in time, we require $2n$ initial conditions to solve the system. The Hamiltonian formulation seeks a first order formulation, which necessitates increasing the size of the system to $2n$. Each initial condition corresponds to an explicit degree of freedom. It is simple to turn Lagrange's equations into a first order system by introducing a differential equation of the sort $v_i = \dot{q}_i$. This is a common way to carry out numerical integration of second order systems. The new variable v_i represents a new degree of freedom that removes a time derivative from the governing equations. Hamiltonian mechanics seeks to do this, but instead of velocities as the new coordinate, we want the

generalized momenta. The state of the system at any instant in time is then the set of position and generalized momenta. Essentially, we need to change coordinates from the Lagrangian construction $L(q_i, \dot{q}_i, t)$ to a new quantity $H(q_i, p_i, t)$ which obeys a new set of $2n$ first order differential equations. To this end, we introduce the Legendre transform. For a function of two variables $f(x, y)$, we have

$$df = \frac{\partial f}{\partial x}dx + \frac{\partial f}{\partial y}dy = udx + vdy$$

We want to change variables from (x, y) to (u, y). Introduce the new function

$$g = f - ux \implies dg = df - udx - xdu = vdy - xdu$$

Given that the differential of g is also

$$dg = \frac{\partial g}{\partial u}du + \frac{\partial g}{\partial y}dy$$

we have that

$$x = -\frac{\partial g}{\partial u}, \quad v = \frac{\partial g}{\partial y}$$

Apparently, the Legendre transforms use is that taking differentials of the new function g eliminates dependence on the variable x which we are seeking to eliminate. The differential dx is replaced with the differential of the new variable du. Thinking about the meaning of this in the context of the Lagrangian, it is tempting to think that if we know how to write the conjugate momenta in terms of the positions and velocities, we could simply plug this into the Lagrangian. The problem is that we are still taking derivatives with respect to the velocities not the momenta. The Legendre transform replaces derivatives w.r.t. the "velocity" variable x with the new "momentum" variable u. Thus, the problem is fully formulated in terms of position and momentum. Turning to the mechanics problem, we take the negative of the Legendre transform given above to write the Hamiltonian as

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

Here, $\dot{q}_i$ plays the role of x and $\frac{\partial L}{\partial \dot{q}_i} = p_i$ plays the role of $u = \frac{\partial f}{\partial x}$. Using the relations spelled out in the beginning, the differential of the Lagrangian is

$$dL = \dot{p}_i dq_i + p_i d\dot{q}_i + \frac{\partial L}{\partial t}dt$$

This means that the differential of the Hamiltonian is

$$dH = \frac{\partial H}{\partial q_i}dq_i + \frac{\partial H}{\partial p_i}dp_i + \frac{\partial H}{\partial t}dt = \dot{q}_i dp_i - \dot{p}_i dq_i - \frac{\partial L}{\partial t}dt$$

Differentials with respect to $\dot{q}_i$ have been removed with the Legendre transform. Equating the two forms of the differential, the governing equations are

$$\dot{q}_i = \frac{\partial H}{\partial p_i}, \quad -\dot{p}_i = \frac{\partial H}{\partial q_i}, \quad -\frac{\partial L}{\partial t} = \frac{\partial H}{\partial t}$$

It can be shown that in many situations, the Hamiltonian is the total energy of the system. In these cases (and perhaps in others), it is possible to write the Hamiltonian explicitly in terms of the generalized position and momenta without resorting to the Lagrangian. Thus it is clear how to take the derivatives of the Hamiltonian in terms of momenta even when the Hamiltonian is constructed in terms of the Lagrangian where the momenta do not appear. We can consider an example from linear elasticity as an attempt to demonstrate this. Call the discretized displacement degrees of freedom q_i. The Lagrangian is

$$L = T - V = \frac{1}{2} M_{ij} \dot{q}_i \dot{q}_j + F_i q_i - \frac{1}{2} K_{ij} q_i q_j$$

The conjugate momenta are

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

Using this definition, the Hamiltonian is then

$$H = \dot{q}_i p_i - \frac{1}{2} \dot{q}_i p_i - F_i q_i + \frac{1}{2} K_{ij} q_i q_j$$

We can also write $\dot{q}_i = M_{ij}^{-1} p_j$ to fully eliminate the velocity degrees of freedom. The Hamiltonian can be written fully in state space as

$$H = \frac{1}{2} M_{ij}^{-1} p_i p_j - F_i q_i + \frac{1}{2} K_{ij} q_i q_j$$

The only explicit time dependence of the problem shows up in the force vector $F_i(t)$. The third of the governing equations then says that

$$\frac{\partial H}{\partial t} = -q_i \frac{\partial F_i}{\partial t}$$

which says that the rate of change of energy of the system is the power input from the forcing. If there were no forcing, or a static forcing, this equation would tell us that energy is conserved. The other two equations for the state are

$$\dot{q}_i = M_{ij}^{-1} p_j, \quad \dot{p}_i = F_i - K_{ij} q_j$$

The second equation is a force equation (rate of change of momentum). As expected, the force is the balance between the applied load and the elastic forces in the system. One benefit of the Hamiltonian formulation is that conservation equations pop out more naturally. Any coordinate (whether position or momentum) ξ_i which does not appear in the Hamiltonian will have a corresponding governing equation

$$\frac{\partial H}{\partial \xi_i} = 0 = \dot{\xi}_i$$

This says that its value is constant in time and it is a conserved quantity. A coordinate which does not appear in the Lagrangian or Hamiltonian is thought of as a symmetry, because changing its value does not change the corresponding energy functional. Thus, symmetries in systems lead to conserved quantities, and the Hamiltonian is particularly convenient for showing this because the problem is formulated explicitly in terms of the position and momenta as independent variables.

2 Liouville Theorem and Equation

The Liouville Theorem is an interesting result from Hamiltonian mechanics which says that a region containing a set of initial conditions in phase space does not change volume under the evolution of the dynamics. The Liouville equation is an analogous result which provides a method for evolving forward in time a probability distribution over initial conditions. Surprisingly, techniques from fluid mechanics are extremely useful for deriving and making sense of all of this. To make things simple, consider a simple harmonic oscillator governed by the Hamiltonian

$$H = \frac{1}{2m}p^2 + \frac{1}{2}kq^2$$

Phase space is a plane describing possible configurations of position and momentum. We ask the following question: how does the area of an initial region in phase space, called Ω_0, change in time when the initial states it encloses are evolved according to the system dynamics? Mathematically, we can write

$$\frac{\partial}{\partial t}\int_{\Omega(t)} d\Omega$$

This is the time rate of change of the area, where $\Omega(t)$ is the area corresponding to Ω_0 evolved forward with Hamilton's equations of motion. We can use the Leibniz rule and the divergence theorem to write this integral as

$$\frac{\partial}{\partial t}\int_{\Omega(t)} d\Omega = \int_{\partial\Omega} \begin{bmatrix}\dot{q}\\ \dot{p}\end{bmatrix} \hat{n} dS = \int_{\Omega} \begin{bmatrix}\partial/\partial q\\ \partial/\partial p\end{bmatrix} \cdot \begin{bmatrix}\partial H/\partial p\\ -\partial H/\partial q\end{bmatrix} d\Omega = 0$$

We have used the equations of motion to derive this result. This states that the volume in phase space occupied by a particular set of systems (defined by their initial conditions) is constant in time. It is interesting to think about this what means for chaotic systems, where very small differences in initial conditions lead to dramatically different solutions. This is the Liouville theorem. To derive the Liouville equation, we now imagine that a probability density exists over a set of initial conditions. We can say that

$$\frac{D}{Dt}\int_\Omega \rho d\Omega = 0$$

When the region Ω follows material particles, the time varying region will always enclose all of the the systems it started with, and thus all the probability density. We can actually use the Reynold's transport theorem to say that

$$0 = \frac{D}{Dt}\int_\Omega \rho d\Omega = \int_\Omega \frac{\partial \rho}{\partial t} + \begin{bmatrix}\partial\rho/\partial q \\ \partial\rho/\partial p\end{bmatrix} \cdot \begin{bmatrix}\dot{q} \\ \dot{p}\end{bmatrix} d\Omega$$

Using the equations of motion and localizing the integral (a valid collection of material particles is a single particle), we obtain

$$\frac{\partial \rho}{\partial t} + \left(\frac{\partial H}{\partial p}\right)\frac{\partial \rho}{\partial q} - \left(\frac{\partial H}{\partial q}\right)\frac{\partial \rho}{\partial p} = 0$$

This is a partial differential equation defined over state space for the evolution of the probability density. The initial condition is simply the initial probability density $\rho(p, q, 0) = \rho_0(p, q)$. It is not clear (to me!) what the boundary conditions are. For the simple harmonic oscillator, this equation becomes

$$\frac{\partial \rho}{\partial t} + \frac{p}{m}\frac{\partial \rho}{\partial q} - kq\frac{\partial \rho}{\partial p} = 0$$

This is a linear partial differential equation with "spatially varying" coefficients. Solving this equation gives the distribution over system states over time. In a sense, this PDE solves a differential equations corresponding to all the points (initial conditions) contained in Ω_0 simultaneously. We think of the probability density as a quantity that is carried along with the "flow" of the systems through state space, analogous to a dye dropped in a fluid flow. Thinking in terms of physical flows seems to be a helpful way to build up intuition for these concepts.