Lecture Notes
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(July 2009)

I. POSTMODERN CLASSICAL MECHANICS

A. Newtonian Mechanics

Classical mechanics, made known to us by Isaac Newton, is useful in describing the motion of macroscopic bodies such as the parabolic motion of a baseball coming off of the bat of Mark McGuire, the kinetics of roller coasters, and the revolution of the planets around our sun. All of these motions can be described by position and velocity (x, v) in the fundamental equations of motion:

$$\dot{x} = v \tag{1.1a}$$

$$\dot{v} = F/m \tag{1.1b}$$

where

$$F(x) = -dV(x)/dx \tag{1.2}$$

e.g. for a Harmonic Oscillator:

$$V(x) = \tfrac{1}{2}kx^2 \tag{1.3}$$

which describes the oscillatory motion of a particle driven by (or responding to) a linear force. That is, the force is always k times its displacement from the origin $|x|$, in the direction toward the origin. You may have seen this before as the small-angle approximation to the pendulum. We'll see this simple potential many times in the rest of the course. Why? Because it is so simple that one can actually solve it! And we can shape many problems, such as the pendulum, to look like a Harmonic Oscillator.

B. Hamiltonian Mechanics

Instead of the position and velocity dependence in Newton's equations of motion, Hamilton's equations of motion depend on position and *momentum* (x, p):

$$\dot{x} = p/m \quad (= mv/m = v) \tag{1.4a}$$

$$\dot{p} = F \quad (= m\dot{v} = F) \tag{1.4b}$$

The space of (x, p) is called **phase space**, and is twice as large as the position space often called **configuration space**. NOTE: Total momentum is conserved, velocity is not. $\Rightarrow p$ is more fundamental than v.

Moreover, the velocity in Eq. (1.4a), may be written as:

$$\frac{p}{m} = \frac{d}{dp}\frac{p^2}{2m} \tag{1.5}$$

where $\frac{p^2}{2m}$ is the kinetic energy, AND the force in Eq. (1.4a) may be written as

$$F = -dV/dx \tag{1.6}$$

where V is the potential energy. Therefore, we can define a quantity, $\mathcal{H}$, such that,

$$\mathcal{H} = \text{Kinetic} + \text{Potential} = \text{Total Energy} \equiv E \ ,$$

with which the equations of motion can be summarized by the so-called Hamilton-Jacobi equations:

$$\dot{x} = \frac{d}{dp}\frac{p^2}{2m} \Rightarrow \dot{x} = \frac{d}{dp}\mathcal{H} \tag{1.7a}$$

$$\dot{p} = \frac{-d}{dx}V(x) \Rightarrow \dot{p} = \frac{-d}{dx}\mathcal{H} \tag{1.7b}$$

Notice that we can get away with this because p is independent of x, and V is independent of p!

And we remember from Newtonian mechanics that E is conserved when the system feels no time-dependent forces. Let's check this. If E is conserved, then its time derivative must be zero. **Why?**

The calculation is as follows:

$$\frac{d\mathcal{H}}{dt} = \frac{d}{dt}\left(\frac{p^2}{2m} + V(x)\right) \tag{1.8a}$$

$$= \frac{p}{m}\frac{dp}{dt} + \frac{dV}{dx}\frac{dx}{dt} \tag{1.8b}$$

Substitution by Hamilton's equations then leads to:

$$\Rightarrow \frac{d\mathcal{H}}{dt} = \frac{p}{m}\left(-\frac{dV}{dx}\right) + \left(\frac{dV}{dx}\right)\frac{p}{m} = 0 \tag{1.8c}$$

Therefore, $\mathcal{H}$ does not change with time $\Rightarrow$ E is conserved!

If the Hamiltonian representation were always as simple as described above, then it would simply be a curious mathematical trick. However, it turns out that the equations of motion described above are fundamental (canonical) in the sense that even in non-conserved systems and/or those in which the Hamiltonian is not separable with respect to position and momentum, the Hamilton-Jacobi equations are still the correct equations of motion!
CONCLUSIONS:

1. In conserved systems — *i.e.*, those which are closed with respect to energy transfers — the Classical Hamiltonian is the Classical Energy. It is conserved, by construction.

2. If you know $\mathcal{H}$, then you know the Classical Equations of motion (1.1).

3. **ASIDE:** Because of the invariant (canonical) nature of the Hamiltonian, it turns out that it is also the fundamental quantity which is quantized in creating Quantum Mechanics.

Note on notation: So far, we have been using x to denote position. Sometimes q is used to denote position as well. In some texts, x and q are used to distinguish between positions in different phase space representations. We will not bother with this distinction.

C. Canonical Transformations

The discussion above should be mostly review from your undergraduate physics courses. Here we introduce a few more fundamental concepts that may or may not be review.

It turns out that it is very useful to be able to view the mechanics of classical mechanics as a series of transformations in phase space. This is an **algebraic** interpretation and it mirrors your **geometric** intuition in that every motion (including those which contain some symmetry) can be represented by a corresponding algebraic transformation. (**QM ASIDE:** Similarly, Quantum Mechanics can be viewed as a theory of transformations on the Hilbert Space. For example, you may recall group theory from physical chemistry: every symmetry in the point topology gives rise to an algebraic symmetry element which preserves the Hamiltonian under orthogonal transformations.)

In terms of solving the classical system, the object then is to discover a phase space transformation which gives you a Hamiltonian which is easy to solve. (We may argue what "easy" means. You will find that it generally means that it is bilinear in terms of the positions and momenta in the new phase space.) But not all transformations of the phase space can be allowed because we need the Hamilton-Jacobi equations to be satisfied. Hence we define a **canonical transformation** of the phase space as one for which the Hamilton-Jacobi equations of Eq. (1.7) are preserved in terms of the transformed Hamiltonian. Such transformations do exist. Two examples of canonical transformations are:

- All transformations on the configuration space alone, *i.e.* those for which x and p are not mixed. These are often called **point transformations**.
- All evolutions of the phase space variables correspond to canonical transformations.

(**QM ASIDE:** This is exactly in parallel to what you do in quantum mechanics where you seek an orthogonal transformation which diagonalizes the Hamiltonian. Given a diagonal Hamiltonian, it is easy to write it's time-dependent solution.)

D. The Lagrangian and Legendre Transformations

The fundamental quantity in Newtownian mechanics is the Lagrangian,

$$\mathcal{L} = \tfrac{1}{2}mv^2 - V(x) \,, \tag{1.9}$$

and it is defined over the (x, v) space. Newton's equations of motion can be rewritten in the obscure fashion:

$$\frac{\partial \mathcal{L}}{\partial x} = \frac{\partial}{\partial t}\frac{\partial \mathcal{L}}{\partial v} \,, \tag{1.10}$$

which is known as the Euler-Lagrange equation. All point transformations automatically preserve the form of the Euler-Lagrange equations. (In fact, you could prove that point transformations are canonical by simply showing that the Euler-Lagrange equations are preserved, and that this in turn implies that the Hamilton-Jacobi equations are preserved.) However, the structure of the Euler-Lagrange equation can change under general canonical transformations because v depends on the mass and this changes through the transformation. This is another reason why we prefer (x, p) phase space coordinates.

To transform from the Lagrangian system to the Hamiltonian system, we use the Legendre Transformation:

$$\mathcal{H}(p,q) = p\dot{q} - \mathcal{L}(v,q) \ . \tag{1.11}$$

This is the same type of transformation that you use in thermodynamics to transform between different free energies. You should convince yourself that from this relation, and the Euler-Lagrange equation, you can, indeed recover the Hamilton-Jacobi equations described above in Eq. (1.7).

As an aside, look again at the Hamilton-Jacobi equations. Note that except for a trivial minus sign, the position and momentum appear in a similar way. It is the similarity of this structure which allows us to consider not only point transformations, but also those which mix position and momentum. That is, these equations of motion treat position and momentum in the same footing, and hence when we try to solve them, we don't have to treat either of them in a special way.

E. The Action

Given a path on the phase space over the time interval (t_0, t_1), we can define Hamilton's Principal function — *vis-a-vis* the action to be,

$$S[p(\cdot), x(\cdot)] = \int_{t_0}^{t_1} \mathcal{L}[p(t), x(t)]dt \ . \tag{1.12}$$

Notice the the action S depends not on a specific value, but rather on a **path**. Think of a path as a function which takes on values in the phase space and is parametrized by the time interval. An object that depends on a function or path over some nontrivial domain is known as a **functional**. A functional is thus a map from a space of functions to a *field*. (Note: This is not a path integral. We'll talk about path integrals later. But for now, think of a path integral as an integral of a functional over a space of paths.) The action, as defined above, is properly defined for any path in the phase space regardless of whether or not the path is generated by the classical equations of motion. The latter much smaller set of paths are called the **classical paths**.

It turns out that classical paths do have a special property with respect to the action: All paths for which the action is a local or global minimum (or even an extremum), are classical paths. As you may recall, a function is extremized at a point if and only if the variation or first derivative at said point is zero. In the same sense, the variation or the functional derivative must be zero for those paths which are extrema of the functional. To make this precise we would need to define a functional derivative, but that would take us too far afield. For now, what you need to know is that the Euler-Lagrange equation is recovered when you set the functional derivative to zero, and as such any path which is a minimum of the action necessarily satisfies the Euler-Lagrange equation. Since it satisfies the Euler-Lagrange equation, it must be a classical path.

The notion that classical paths are the solution which minimizes the action is known at the **Least Action Principle** or more precisely the **Extremal Action Principle**. What happens in quantum mechanics is that the non-classical paths also contribute! In this sense, we would have the beginnings of a fundamental quantum mechanics if only we knew how to weigh our paths —*viz.*, if we could figure out how much each path should contribute.

Feynman found the clue to answering this puzzle in Dirac's book on the "Principles of Quantum Mechanics," and built upon it in developing the path integral description of quantum mechanics. Moreover, this same type of thinking is necessary in developing quantum mechanical **partition functions** in statistical mechanics. In this course, though, we will treat only classical partition functions.

F. Numerical Integration of Equations of Motion

This section could also be titled "Molecular Dynamics" (MD) in cases where we attempt to solve the classical equations of motion for a system of molecules and/or atoms. At least this would be so in an ideal world. Unfortunately, in order to do this we need to presuppose a certain type of potential, *i.e.*, we need to know the Hamiltonian before we can integrate its corresponding Lagrangian equations! Many authors implicitly assume a particular construction of this Hamiltonian when they use the term "MD," and this sometimes leads to confusion. (In fact, it is sometimes useful to use non-physical Hamiltonians!) In our course, MD will simply mean that given some Hamiltonian, we will propagate the system from some initial time to some final time. The Hamiltonian may correspond to a multi-dimensional system with N degrees of freedom. And N may be very, very large. If N is on the order of 1000's, we may be able to calculate at most a few picoseconds of such a trajectory on the computer...

The question that we wish to address here is how to calculate said trajectory, given that there exists a function/subroutine which provides the force at any desired point. The general idea is that if we know the velocity-phase space point, $[x(t), v(t)]$, at some time t, we need to obtain the new phase space point $[x(t+\tau), v(t+\tau)]$ at some later time $t+\tau$ with a reasonable amount of accuracy. By iterating this procedure, we can then obtain the phase space point at arbitrary times. Looking at Eq. (1.1), and remembering the infinitessimal definition of derivatives,

$$x(t+\tau) \approx x(t) + \tau v \tag{1.13a}$$

$$v(t+\tau) \approx v(t) + \tau F/m \ , \tag{1.13b}$$

The approximation is clearly here because for any finite τ, the difference between the phase space points will include higher order terms in τ. You should also notice that we did not specify the time at which to evaluate v and F/m, *i.e.*, the first order correction. In principle, any choice of time within the interval would be correct in so far as the error would still be of second order. However, there may be some choices that are better in the sense that the coefficient in front of the second order term may be smaller, and this leads to better accuracy at larger time steps. To specifically program the MD algorithm, we would need to make this choice explicit. For these details, you should look at the Allen and Tildesley reference below, noting that the velocity-verlet algorithm is presently the most popular choice.

Although Eq. (1.13), may seem to be one-dimensional, it is also the correct structure for the multi-dimensional case. The only added wrinkle is that the force F which is obtained at the value of the position at the chosen time within the time interval (as described above), is now evaluated at the multi-dimensional position. This is the origin of the coupling between the particles.

Finally, it should be clear that any method which provides the solution of a family of N first-order partial differential equations may be used to obtain the classical trajectories.

For example, one could use Runge-Kutta and/or Gear methods. However, the approach described above works particularly well for the family of classical Hamiltonians because it is reasonably accurate, and requires a relatively small number of potential evaluations. The latter is important because for a multi-dimensional system, it is often very time consuming to evaluate the potentials leading to the force at each time step.

G. References

The following is meant to provide a representative set of references, but it is by no means all-inclusive:

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8. M. P. Allen and D. J. Tildesley, *Computer Simulation of Liquids* (Oxford, New York, 1987).

9. D. Frenkel and B. Smit, *Understanding Molecular Simulation From Algorithms to Applications* (Academic Press, San Diego, 2001), 2nd edition.