10 Lecture 10: Classical mechanics: review

Newton realized that if we know the current position x and velocity $\dot{x}$ of a point mass, its future (and its past) is completely determined. This is called the Newton-Laplace principle of determinacy. This means its acceleration $\ddot{x}$ is determined by x and $\dot{x}$. The resultant ODE is called Newton's equation of motion.

Since every graduate student should be very familiar with the practical use of classical mechanics, in this lecture, I concentrate on topics that are not very widely known or not so much stressed:
(1) How to construct a variational principle,
(2) When the variational principle is actually a minimization principe,
(3) A succinct demo of the Jacobi identity for Poisson brackets.
(4) How Schrödinger 'used' the Hamiltonian principle to derive his equation.

10.1 Newton-Laplace Principle of Determinacy[110]

The principle asserts that the state (= point in the phase space) of a mechanical system (= everything from Newton's and Laplace's point of view) at any fixed moment of time t uniquely determines all of its (future and past) states:

From $x(t_0)$ and $v(t_0) = \dot{x}(t_0)$, $(x(t), v(t))$ for all t is uniquely determined.

In particular, we can calculate the acceleration as

$$\ddot{x} = f(x, \dot{x}, t). \tag{10.1}$$

This is known as Newton's equation of motion. With time-reversal symmetry there is no first order derivatives in the equation

$$\ddot{x} = f(x, t). \tag{10.2}$$

Thus, to describe the system mechanics is to provide f, the force (experimentally). As noted in the preface to *Principia*, for Newton to find f for various phenomena was the core physics. This idea hindered the kinetic theory of gasses to explain the gas pressure.

The equivalence of Newton's equation of motion and the principle of determinacy is shown by the unique existence theorem of the solution for the ODE (see **3.18**).

[110] The following paper proposes to use the halting problem to deny the existence of Laplace's demon: Josef Rukavicka, Rejection of Laplace's Demon. Am Math Month 121 498 (2014). Basically, the question is: what is the significance of undecidable questions in this context?

Thus it is not unconditional, but as long as the motion is sufficiently smooth the equivalence is guaranteed.

Newton introduced the concept of 'force' and established the law of universal gravitation (with superposition principle).

10.2 Determinacy implies predictability?

One of the key issues of nonlinear dynamics is to make it clear that the answer to the question is negative: even though deterministic you cannot predict the future of the system, because the indefiniteness (error) in the intial condition could be exponentially magnified within a short time span.

There are, however, actually, more serious reasons why determinacy cannot generally imply predictability. One is already mentioned in the footnote of **10.1**: for example, the calculation needed to predict the future may not end. I do not know whether we can make a natural-looking ODE example for this. In this case whether computation can actually produce a number or not is the issue; we cannot even predict whether the computer will eventually give the answer or not. The other case of unpredictability is that the computer can indeed produce numbers, but their reliability (i.e., the size of the error bar) are never guaranteed.

10.3 Variational principle

The fundamental equation of mechanics is (10.2), but why is this form? Is there any deeper reason (yes, rational reason) for the Creator to choose this law?[111] Somehow, the law should be 'optimized', a natural route to variational principles. In elementary classical mechanics we have already learned Lagrange's principle, but here let us construct the variational principle from (10.2). We use

Theorem [Veinberg][112] Suppose

[111] This is exactly the 'naturalness' question (used in high energy physics). C. Lanczos, *The variational principle of mechanics* (University of Toronto Press, 3rd ed., 1960) Preface says, "There is hardly any other branch of the mathematical sciences in which abstract mathematics speculation and concrete physical evidences go so beautifully together and complement each other so perfectly." It is a good lesson to know that mathematical beauty does not guarantee the correctness of a theory in natural science. It is very often the case that what we believe natural is not actually naturally realized in Nature; to recognize this may be a sign of a true progress.

[112] See R. W. Atherton and G. M. Homsy, On the existence and formulation of variational principle for nonlinear differential equations, Studies Appl. Math. **LIV**, 31 (1975). For ODE there is a newer paper: I. A. Anderson and G. Thompson, The inverse problem of the calculus of variation for ordinary differential equations, Memoir AMS **98**, Number 473 (1991).

(1) N is an operator from a Hilbert space $\mathcal{H}$ into its conjugate space,
(2) N has a linear Gateau derivative[113] $DN(u,h)$ at every point of the ball $B = \{u \,|\, \|u - u_0\| < r\}$ and for any $h \in \mathcal{H}$,
(3) The scalar product $\langle h_1, DN(u,h_2)\rangle$ is continuous at every point of the ball B for any $h_1, h_2 \in \mathcal{H}$.
Then, a necessary and sufficient condition for $N(u) = 0$ to be the Euler-Lagrange's equation of a variational principle in the ball B is the symmetry

$$\langle h_1, DN(u,h_2)\rangle = \langle h_2, DN(u,h_1)\rangle. \tag{10.3}$$

The variational functional $F(u)$ is given by

$$F(u) = -\int dt \int_0^1 d\lambda\, u(t) N(\lambda u(t)). \tag{10.4}$$

You should have realized a perfect parallelism between the condition for a force $\boldsymbol{F}$ to be conservative: curl$\boldsymbol{F} = 0$ and the above theorem.

10.4 Application to Newton's equation of motion

(10.3) implies (exercise!) that f cannot depend on $\dot{x} = v$ (that is, imposing the variational principle enforces time-reversal symmetry) and the force must be conservative. Under these conditions we obtain (exercise!) the usual result we know: the variational functional is A called the action:

$$A = \int dt\, L, \tag{10.5}$$

with

$$L = T - V, \tag{10.6}$$

called the Lagrangian, where T is the kinetic energy and V the potential energy. The equation of motion obtained from $\delta A = 0$ (the action principle) reads (Lagrange's equation of motion), as you know well,

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{x}} - \frac{\partial L}{\partial x} = 0. \tag{10.7}$$

[113] ⟪**Gateau derivative**⟫ This is a functional-derivative counterpart of the directional derivative, and is also called the weak derivative. Let $F : X \to Y$, where X and Y are normed space. Then,

$$DF(x,h) = \frac{d}{dt}F(x+th)\bigg|_{t=0}.$$

Remark on the Lagrangian:
(0) Landau-Lifshitz, *Mechanics* Chapter 1 is the best practical introduction.
(1) L is not unique; we may add any total derivative wrt time. This allows more general transformations than the ordinary coordinate changes (called canonical transformations (Lecture 13)).
(2) T is always a quadratic form of $\dot{x}$.

10.5 Action minimum principle

The variational principle itself does not care whether A is minimum or not along the actual motion, but the founding fathers of the principle clearly expected 'minimization.' This is actually true as long as the path is not too long. Precisely put, until the stationary curve hits the conjugate point, the minimum principle is true.

10.6 Conjugate point

Consider two actual trajectories going through a point A making a small angle with each other. If these two trajectories cross with each other at B, it is called a conjugate point of A (see Fi.g 10.1).

If the final point is reached from the initial point before reaching its conjugate point, the action is actually minimum.

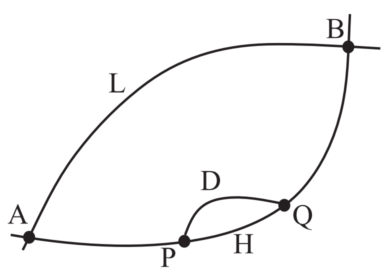

Figure 10.1: A conjugate point. Here, trajectories L and H both satisfy the variational principle.

[Demo] In Fig. 10.1 trajectories L and H both satisfy the variational principle, starting from A with different directions, and then cross for the first time at B (a conjugate point of A). Suppose APHQB is not an actual trajectory. If PHQ is not the actual trajectory, then there must be an actual one PDQ. Since we can choose Q sufficiently close to P,[114] **10.7** tells us the action along PDQ

[114] Suppose PHQ is not an actual path. Take R on this path. If PR is an actual path, we can choose replace PHQ with RHQ. If PR is not actual, there must be a 'bypass' which is the actual path.

is smaller than that along PHQ. Then, $\delta^2 A < 0$ on PDQ, contradicting the assumption that $\delta^2 A = 0$ along PHQ.

10.7 Locally, action principle is minimum principle

We first rewrite the action principle in the form of Maupertuis (1698-1759)'s principle (= the action principle on the constant energy E surface):

$$A = \int_{t_0}^{t_1} dt\,(T - V) = \int_{t_0}^{t_1} dt\,(2T - E) = 2\int_{t_0}^{t_1} dt\,T - E(t_1 - t_0). \tag{10.8}$$

This means we have only to consider the first term as the action (denoted as A'). Since T is quadratic wrt $\dot{q}$, where q is the spatial coordinate, we may write $T = A_{ij}\dot{q}_i\dot{q}_j/2 = A_{ij}dq_idq_j/2dt^2$ (summation convention implied), so

$$dt = \sqrt{A_{ij}dq_idq_j/2T} \tag{10.9}$$

Therefore,

$$A' = 2\int_{t_0}^{t_1} dt\,T = \int_{s=t_0}^{s=t_1} ds\,\sqrt{2(E - V)}\sqrt{A_{ij}q_i'(s)q_j'(s)}. \tag{10.10}$$

Now, we must study $\delta^2 A'$. We vary the trajectory as $q \to q + \delta q$. Choose the time range $[t_0, t_1]$ sufficiently small so the variation δq is much smaller than $\delta q'$. Therefore, we have only to consider the second $\sqrt{\cdots}$ in (10.10). This is a (positive definite) quadratic form, so its stationary value must be minimum.

10.8 Legendre transformation $L \to H$

We know Lagrange's equation of motion means the following 1-form:

$$dL = p d\dot{q} - \frac{\partial V}{\partial q} dq, \tag{10.11}$$

where q are spatial coordinates, and p the momenta. Now we apply the following Legendre transformation

$$H = \sup_{\dot{q}}[p\dot{q} - L] = T + U. \tag{10.12}$$

H is called the Hamiltonian and

$$dH = \dot{q}dp + \frac{\partial V}{\partial q} dq \tag{10.13}$$

implies the Hamilton's equation of motion (= the canonical equation of motion)

$$\dot{q} = \frac{\partial H}{\partial p}, \ \frac{\partial V}{\partial q} = \frac{\partial H}{\partial q} = -\dot{p}. \tag{10.14}$$

10.9 Hamilton's principle.
Since $L = \sum p_i \dot{q}_i - H$ (**10.8**), the action principle **10.4** may be rewritten as

$$\delta \int \left[\sum_i p_i \dot{q}_i - H \right] dt = 0. \tag{10.15}$$

Regarding p and q to be independent variables, we obtain directly the canonical equation of motion (10.14) (use integration by parts). The resultant variational principle (10.15) is called *Hamilton's principle.*

10.10 Poisson bracket.
Let f and g be differentiable phase functions (functions of q and p). We introduce the *Poisson bracket* $[f, g]_{PB}$[115] as

$$[f, g]_{PB} \equiv \frac{\partial f}{\partial q}\frac{\partial g}{\partial p} - \frac{\partial g}{\partial q}\frac{\partial f}{\partial p} = \sum_i \left(\frac{\partial f}{\partial q_i}\frac{\partial g}{\partial p_i} - \frac{\partial g}{\partial q_i}\frac{\partial f}{\partial p_i} \right). \tag{10.16}$$

10.11 Canonical equation of motion in terms of Poisson brackets
(10.14) reads

$$\dot{q}_i = [q_i, H]_{PB}, \quad \dot{p}_i = [p_i, H]_{PB}. \tag{10.17}$$

Thus, the canonical equations of motion for q and p have become symmetric. (cf. Heisenberg's equation of motion in QM)

10.12 Properties of Poisson bracket
Note the following general relations:

[115] or simply, $[f, g]$ when quantum and classical mechanics do not appear simultaneously.

(i) $[f, g]_{PB} = -[g, f]_{PB}$.
(ii) $[f, g+h]_{PB} = [f, g]_{PB} + [f, h]_{PB}$.
(iii) $[cf, g]_{PB} = c[f, g]_{PB}$, where c is a constant.
(iv) [*Jacobi's identity*] $[f, [g, h]_{PB}]_{PB} + [g, [h, f]_{PB}]_{PB} + [h, [f, g]_{PB}]_{PB} = 0$.

(i)-(iv) imply that the Poisson bracket defines a *Lie algebra* structure for the set of the differentiable phase functions. (i)-(iii) are easy to show. (iv) implies that $[\ ,\ ]_{PB}$ is not associative. Usually showing (iv) requires almost brute force lengthy calculation, but see at the end of this item.

Notice further that
(v) $[fg, h]_{PB} = f[g, h]_{PB} + [f, h]_{PB}g$.
(vi) If f and g depend on a parameter α differentiably, then $d[f, g]_{PB}/d\alpha = [df/d\alpha, g]_{PB} + [f, dg/d\alpha]_{PB}$.
(vii) Let F be a function of phase functions f_i. Then $[F, g]_{PB} = (\partial F/\partial f_i)[f_i, g]_{PB}$.

Notice that for any differentiable phase function h, we can define a one parameter group defined by $df/d\alpha = [f, h]_{PB}$ (actually this is called an infinitesimal canonical transformation and h its generator; see **13.4**). Use this to (vi) (compute $d[f, g]/d\alpha$), and we get Jacobi's identity (iv) immediately.

10.13 Integral of motion; conservation of energy

An *integral of motion* Q is a phase function which is time-independent. (10.17) implies

$$[Q, H]_{PB} = 0, \tag{10.18}$$

if Q does not have any explicit time dependence.
Obviously,

$$[H, H]_{PB} = 0. \tag{10.19}$$

This is the conservation of (mechanical) energy (H must be t-independent).

10.14 Poisson brackets of various quantities

We can easily demonstrate

$$[p_i, p_j]_{PB} = 0, \quad [q_i, q_j]_{PB} = 0, \quad [q_i, p_j]_{PB} = \delta_{ij}. \tag{10.20}$$

Here (i, j, k) is a cyclic permutation of $(1, 2, 3)$. We also have for angular momentum L_i

$$[L_i, L_j]_{PB} = L_k, \quad [L_i, p_j]_{PB} = p_k, \quad [L_i, q_j]_{PB} = q_k, \tag{10.21}$$

and other Poisson brackets between angular momentum components and phase variables are zero. More generally, for a differentiable phase function F,

$$[F, p_i]_{PB} = \frac{\partial F}{\partial q_i}, \quad [F, q_i]_{PB} = -\frac{\partial F}{\partial p_i}. \tag{10.22}$$

10.15 Hamilton-Jacobi's equation.

Let us consider the action A defined in **10.4** as a function of the end time t and the end position $q_i = q_i(t)$:

$$A(q, t) = \int_{t_0}^{t} L(q(s), \dot{q}(s), s)ds, \tag{10.23}$$

where L is the Lagrangian. Obviously,

$$\frac{dA}{dt} = L(q_i(t), \dot{q}_i(t), t) = p_i(t)\dot{q}_i(t) - H, \tag{10.24}$$

where H is the Hamiltonian (10.12). Hence,

$$dA = \sum_i p_i dq_i - H dt, \tag{10.25}$$

that is,

$$\frac{\partial A}{\partial q_i} = p_i, \quad \frac{\partial A}{\partial t} = -H. \tag{10.26}$$

Since H is a function of q_i, p_i, and t, we obtain a closed equation for A

$$\frac{\partial A}{\partial t} + H\left(q_i, \frac{\partial A}{\partial q_i}, t\right) = 0. \tag{10.27}$$

This is called the *Hamilton-Jacobi equation*. Note that it does not contain the momentum coordinates. For example, for a particle of mass m in the potential V, the Hamilton-Jacobi equation reads

$$\frac{\partial A}{\partial t} + \frac{1}{2m}\left\{\left(\frac{\partial A}{\partial x}\right)^2 + \left(\frac{\partial A}{\partial y}\right)^2 + \left(\frac{\partial A}{\partial z}\right)^2\right\} + V(x, y, z) = 0. \tag{10.28}$$

10.16 Schrödinger's "Quantization as eigenvalue problem I"[116]

Schrödinger starts with the Hamilton-Jacobi equation (10.27) in the following separated form:

$$H\left(q, \frac{\partial A_0}{\partial q}\right) = E, \tag{10.29}$$

with $A = -Et + A_0$, where A_0 is called Hamilton's principal function. He introduces ψ as

$$A_0 = \hbar \log \psi. \tag{10.30}$$

Schrödinger use the symbol K instead of $\hbar$. Thus, the equation (10.29) now reads

$$(\nabla\psi)^2 - \frac{2m}{\hbar^2}(E-V)\psi^2 = 0. \tag{10.31}$$

Instead of this equality, he replaces the quantization condition with the following variational problem; he says in a footnote that he is aware that this formulation is not necessarily unique:

$$\delta J = \delta \int d^3\boldsymbol{x} \left[(\nabla\psi)^2 - \frac{2m}{\hbar^2}(E-V)\psi^2\right] = 0. \tag{10.32}$$

The resultant equation is (assuming that the wave function vanishes at infinity) the time-independent Schödinger equation.

In this paper, he goes on to solve the hydrogen atom completely (he acknowledges H. Weyl's help). The ad hoc introduction of the Schrödinger equation as outlined above is fully justified by recovering Bohr's energy levels.

[116] Quantisierung als Eigenwertproblem I, Ann. Phys(4) 79, 361-376 (1926): received on January 27, 1926