

MATH4104 Advanced Hamiltonian Dynamics and Chaos.

This is a course on Classical and Quantum Hamiltonian Dynamics. The aim of the first half of the course is to understand the basics of chaos in Classical Hamiltonian Systems. There are a number of techniques, which we will learn about, that can be employed to enable one to analyze and understand the presence of chaos in a given Classical Hamiltonian System.

First we will review Lagrangian and Hamiltonian Mechanics. Then we will look at Canonical Transformations, which are variable transformations that preserve the Hamiltonian structure. These can be used to analyze the resonances in a system. The presence and size of these resonances is a major factor in the level of chaos present. We then look at the KAM theorem, which uses Canonical transformations to prove that in a whole class of systems "KAM tori" limit the extent of the chaos to subregions of the phase space.

To investigate further we look at Twist Maps and in particular the Standard Map, which is a particularly simple twist map that exhibits most of the typical behavior of chaotic maps. At the end of the classical section we will look at some other examples, e.g. chaos in Billiards.

Course Outline

• 1 Classical Dynamics

- 1.1 Lagrangian Mechanics
- 1.2 Hamiltonian Mechanics
- 1.3 Canonical Transformations
- 1.4 Integrable Systems and Action Angle variables
- 1.5 Canonical perturbation Theory
- 1.6 Resonances and the KAM Theorem
- 1.7 Twist Maps
- 1.8 The Standard Map
- 1.9 Chaos Near Homoclinic Orbits
- 1.10 Chaos in Billiards

• 2. Quantum Dynamics

- 2.1 Review of Quantum Theory
- 2.2 Atoms in Optical Potentials
- 2.3 Integrable Nonlinear Quantum Dynamics
- 2.4 Quasi-Integrable Nonlinear Quantum Dynamics
- 2.5 Dynamical Localization
- 2.6 Nonlinear Quantum Maps
- 2.7 Random Matrices
- 2.8 Trace Formulas and Periodic Orbits
- 2.9 Quantum Billiards
- 2.10 Mesoscopic Systems

Reference Books

Random and Stochastic Motion, A.J. Lichtenberg and M.A. Lieberman, Applied mathematical Sciences vol38, Springer Verlag, New York, 1982.

The Transition to Chaos, in conservative classical systems: quantum manifestations. Linder Reichl, Springer Verlag, New York, 1992.

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Quantum chaos : between order and disorder : a selection of papers compiled and introduced by Giulio Casati, Boris Chirikov.

A modern approach to quantum mechanics, Townsend, McGraw-Hill (this is the level of QM assumed).

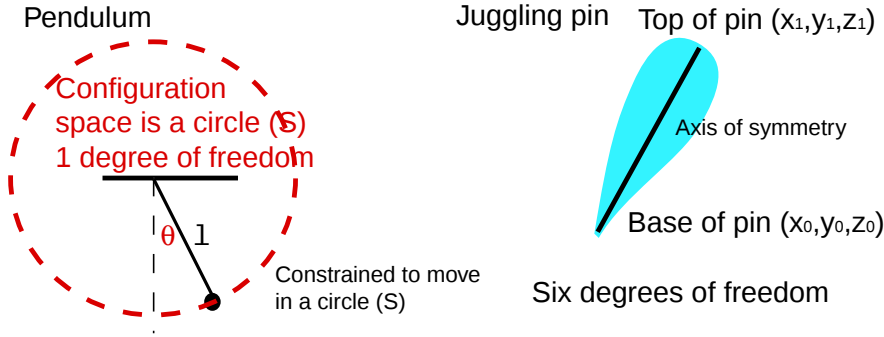
Section 1. Classical Dynamics

Section 1.1 Lagrangian Mechanics

Lagrange devised a general method for obtaining the equations of motion for a wide class of mechanical systems. This included constrained systems. Consider a number of particles P_i with masses m_i and position and velocity vectors $\mathbf{r}_i$ and $\mathbf{v}_i$. Then for an unconstrained system the equations of motion are simply Newton's equations of motion:

$$m_i \dot{\mathbf{v}}_i = \mathbf{F}_i \quad \text{for } i = 1 \dots N, \text{ where } \mathbf{F}_i \text{ is the force acting on the particle } P_i.$$

But typically systems are constrained, for instance a bead on a wire is constrained to move on the wire, or a pendulum bob is a fixed distance from the point of support, in which case there are additional forces which are not simple to work out. But if you use Lagrange's method you never have to work them out.



The simplest type of constraint to imagine is one that constrains the geometry of the system. Think of the pendulum again. In 2D the bob is constrained to move in a circle, so the motion has only one independent variable; θ . The space of possible motion is the circle (S), which is one dimensional. This is called the **Configuration space** of the system S . The trick is to find new variables that reflect the dimension of the **Configuration space**.

- **Generalized coordinates** If the configuration of a system S is determined by the values of a set of independent variables $q_1, q_2, \dots, q_n$ then $\{q_1, q_2, \dots, q_n\}$ is said to be a set of generalized coordinates for S .

Note that the variables $q_1, q_2, \dots, q_n$ must be **independent**, that is there can be no functional relationship connecting them.

Also the variables $q_1, q_2, \dots, q_n$ **determine** the configuration of the system S , so that if the values of $q_1, q_2, \dots, q_n$ are known then the position of every particle of S is determined.

The number of generalized coordinates needed to specify a configuration S is called the **degrees of freedom** of S . But there may be more than one way to choose the generalized coordinates. Suppose there are n of them. Then there are also n **generalized velocities**:

$$\mathbf{q} = (q_1, q_2, \dots, q_n) \quad \dot{\mathbf{q}} = (\dot{q}_1, \dot{q}_2, \dots, \dot{q}_n)$$

Since the actual position of a particle in the space $\mathbf{r}_i$ depends on the generalized coordinates the actual velocity is

$$\mathbf{v}_i = \frac{\partial \mathbf{r}_i}{\partial q_1} \dot{q}_1 + \dots + \frac{\partial \mathbf{r}_i}{\partial q_n} \dot{q}_n = \sum_{j=1}^n \frac{\partial \mathbf{r}_i}{\partial q_j} \dot{q}_j$$

In most cases the **Lagrangian** for a system is defined as the difference between the Kinetic Energy and the Potential Energy of the system.

$$L(\mathbf{q}, \dot{\mathbf{q}}, t) = T(\mathbf{q}, \dot{\mathbf{q}}, t) - U(\mathbf{q}, t)$$

Hamilton's Principle of Stationary Action can then be used to obtain **Lagrange's** Equations of motion. (Note that in this course we will be mainly concerned with systems without dissipation.) First imagine any path in a Configuration space.

Hamilton's Principle of Stationary Action states that

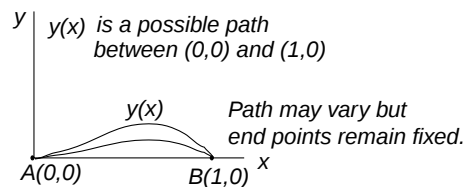
Of all the kinematic motions that take a mechanical system from one given configuration to another within a given time interval, the actual motion is the one that minimizes the time integral of the Lagrangian of the system.

The idea is that physical processes are governed by minimizing principles. In practice this means we need to be able to find stationary functions of, in this case, an integral functional. Minimizing principles result in variational principles, which can be converted to a differential equations by the **calculus of variations**.

Geodesics are a good example of a variational principal because geodesics are the paths of shortest length in some geometry. For a simple example take the points $A = (0, 0)$ and $B = (1, 0)$ in $\mathbb{R}^2$. If $y(x)$ is the path then the length of the path is

$$\ell(y) = \int_0^1 \sqrt{1 + \left(\frac{dy}{dx}\right)^2} dx \quad \text{where } y(0) = 0 \text{ and } y(1) = 0$$

So, for a geodesic, we need to minimize $\ell(y)$ over all possible functions $y(x)$, such that $y(0) = 0$ and $y(1) = 0$.



Calculus of Variations

Consider $J[x] = \int_a^b F(x, \dot{x}, t) dt$.

Suppose that the function $x^*(t)$ minimizes the functional $J[x]$. Then $J[x] \geq J[x^*]$.

Or $J[x^* + h] \geq J[x^*]$ for all admissible variations $h(t)$, with $h(a) = 0$ and $h(b) = 0$.

Now assume that $h(t)$ is small and using calculus

$$J[x^* + h] - J[x^*] = \int_a^b \left[h \frac{\partial F}{\partial x}(x^*, \dot{x}^*, t) + \dot{h} \frac{\partial F}{\partial \dot{x}}(x^*, \dot{x}^*, t) \right] dt + O(\|h\|^2)$$

where for h small the norm is defined as $\|h\| = \max_{a \leq t \leq b} |h(t)| + \max_{a \leq t \leq b} |\dot{h}(t)|$.

The second term can be rewritten by using integration by parts:

$$\int_a^b \dot{h} \frac{\partial F}{\partial \dot{x}}(x^*, \dot{x}^*, t) dt = \left[h(t) \frac{\partial F}{\partial \dot{x}}(x^*, \dot{x}^*, t) \right]_{t=a}^{t=b} - \int_a^b h \frac{d}{dt} \left(\frac{\partial F}{\partial \dot{x}}(x^*, \dot{x}^*, t) \right) dt$$

But $h(a) = 0$ and $h(b) = 0$ so

$$\int_a^b \dot{h} \frac{\partial F}{\partial \dot{x}}(x^*, \dot{x}^*, t) dt = - \int_a^b h \frac{d}{dt} \left(\frac{\partial F}{\partial \dot{x}}(x^*, \dot{x}^*, t) \right) dt$$

This means that

$$J[x^* + h] - J[x^*] = \int_a^b h \left[\frac{\partial F}{\partial x}(x^*, \dot{x}^*, t) - \frac{d}{dt} \left(\frac{\partial F}{\partial \dot{x}}(x^*, \dot{x}^*, t) \right) \right] dt + O(\|h\|^2)$$

Now a local minimum requires $J[x^* + h] - J[x^*] \geq 0$ and because this must be true for all admissible variations $h(t)$ this implies that the integrand is zero:

$$\frac{\partial F}{\partial x}(x^*, \dot{x}^*, t) - \frac{d}{dt} \left(\frac{\partial F}{\partial \dot{x}}(x^*, \dot{x}^*, t) \right) = 0$$

The result is reversible.

• Euler-Lagrange Equation for one degree of freedom

If the function x^* makes the integral functional

$$J[x] = \int_a^b F(x, \dot{x}, t) dt$$

stationary, then x^* must satisfy the **Euler-Lagrange Equation**

$$\frac{\partial F}{\partial x} - \frac{d}{dt} \left(\frac{\partial F}{\partial \dot{x}} \right) = 0.$$

The converse is also true.

For instance take the simple example of the geodesic, where

$$\ell(y) = \int_0^1 \sqrt{1 + \left(\frac{dy}{dx} \right)^2} dx \quad \text{where } y(0) = 0 \text{ and } y(1) = 0$$

and for a geodesic, we need to minimize $\ell(y)$ over all possible functions $y(x)$, such that $y(0) = 0$ and $y(1) = 0$.

$$F(y, \frac{dy}{dx}, t) = \sqrt{1 + \left(\frac{dy}{dx} \right)^2}, \quad \Rightarrow \quad \frac{\partial F}{\partial y} = 0$$

So, using the notation $y' = \frac{dy}{dx}$, the Euler-Lagrange Equation is

$$\frac{d}{dx} \left(\frac{\partial F}{\partial y'} \right) = \frac{d}{dx} \left(\frac{y'}{\sqrt{1 + y'^2}} \right) = 0$$

$$\Rightarrow y' = \frac{dy}{dx} = c \quad \Rightarrow \quad y = cx + d$$

But $y(0) = y(1) = 0 \Rightarrow c = d = 0$, so $y \equiv 0$.

- **Higher degrees of freedom** In an n degree of freedom system $\mathbf{q} \in \mathbb{R}^n$. If the function $\mathbf{q}^*$ makes the integral functional, usually called the **action functional**

$$S[\mathbf{q}] = \int_{t_0}^{t_1} L(\mathbf{q}, \dot{\mathbf{q}}, t) dt$$

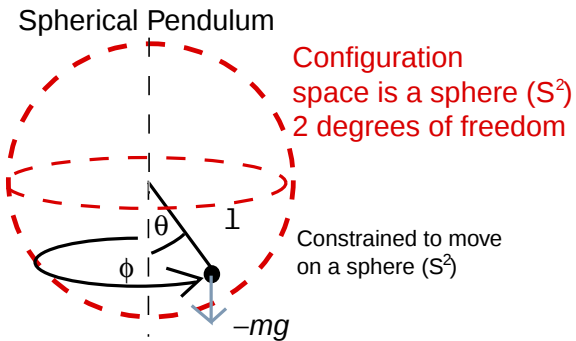
stationary, then $\mathbf{q}^*$ must satisfy the n **Euler-Lagrange Equations**

$$\frac{\partial L}{\partial q_j} - \frac{d}{dt} \left(\frac{\partial L}{\partial \dot{q}_j} \right) = 0. \quad (1 \leq j \leq n)$$

simultaneously.

Using Lagrange's equations is usually straightforward.

Consider the **spherical pendulum**. Using spherical polars, θ and ϕ , as the generalized coordinates, the Lagrangian (the kinetic energy minus the potential energy) is

$$L = \frac{1}{2} m a^2 \left[\dot{\theta}^2 + (\sin \theta \dot{\phi})^2 \right] + m g a \cos \theta$$


Spherical Pendulum

Configuration space is a sphere (S^2)
2 degrees of freedom

Constrained to move on a sphere (S^2)

Lagrange's equations of motion are

$$m a^2 \cos \theta \sin \theta \dot{\phi}^2 - m a^2 \ddot{\theta} = 0 \quad \Rightarrow \quad \ddot{\theta} = \cos \theta \sin \theta \dot{\phi}^2$$

and

$$\frac{d}{dt} (m a^2 \sin^2 \theta \dot{\phi}) = 0 \quad \Rightarrow \quad m a^2 \sin^2 \theta \dot{\phi} = c \quad \text{the axial momentum is conserved.}$$

Kepler's Central Force Problem, with generalized coordinates r the distance between the masses and θ the angle the line between the masses makes with the horizontal.

$$L = \frac{1}{2} \mu (\dot{r}^2 + r^2 \dot{\theta}^2) - U(r), \quad \text{where } \mu = \frac{m_1 m_2}{m_1 + m_2} \text{ is the effective mass}$$

Lagrange's equations of motion are

$$\mu r \dot{\theta}^2 - U' - \mu \ddot{r} = 0 \quad \text{and} \quad \mu r^2 \dot{\theta} = \text{constant of the motion.}$$

One of the remarkable results of Hamilton's principle is that **Lagrange's equations of motion are invariant under transformations of the generalized coordinates.** Suppose we choose new generalized coordinates $\mathbf{q}'$ and so we have a new action functional

$$S[\mathbf{q}'] = \int_{t_0}^{t_1} L(\mathbf{q}', \dot{\mathbf{q}}', t) dt$$

Then the extremals of $S[\mathbf{q}]$ map into the extremals of $S[\mathbf{q}']$ and vice versa. So the equations of motion are invariant.

However **the Lagrangian is not unique**. In fact the addition to the Lagrangian of a *total time derivative* does not change the paths of stationary action.

Consider the total time derivative of $F(\mathbf{q}, t)$

$$\frac{dF(\mathbf{q}, t)}{dt} = \sum_{j=0}^n \frac{\partial F}{\partial q_j} \dot{q}_j + \frac{\partial F}{\partial t}$$

Now suppose that $L' = L + \frac{dF}{dt}$ so that

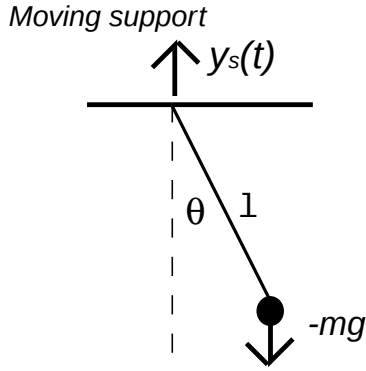
$$S'[\mathbf{q}] = \int_{t_0}^{t_1} L'(\mathbf{q}, \dot{\mathbf{q}}, t) dt = \int_{t_0}^{t_1} L(\mathbf{q}, \dot{\mathbf{q}}, t) dt + \int_{t_0}^{t_1} \frac{dF(\mathbf{q}, t)}{dt} dt$$

But $\int_{t_0}^{t_1} \frac{dF(\mathbf{q}, t)}{dt} dt = [F(\mathbf{q}, t)]_{t_0}^{t_1}$ which will not change under minimization because it is only a function of the end points and the end points do not change as the path is varied. So to minimize $S'[\mathbf{q}]$ we need to minimize $S[\mathbf{q}]$.

It is sometimes useful to use this result and choose a Lagrangian which is not strictly the difference between the kinetic and potential energies.

Take the **Driven pendulum** where the support is moving vertically $y_s(t)$.

$$L = T - V = \frac{1}{2}m(v_x^2 + v_y^2) - mgy$$



Using the generalized coordinate θ as shown

$$L = \frac{1}{2}m \left(\ell^2 \cos^2 \theta \dot{\theta}^2 + \left(\dot{y}_s(t) + \ell \sin \theta \dot{\theta} \right)^2 \right) - mg(y_s - \ell \cos \theta)$$

$$L = \frac{1}{2}m \left(\ell^2 \dot{\theta}^2 + 2\dot{y}_s(t)\ell \sin \theta \dot{\theta} + \dot{y}_s^2 \right) - mg(y_s - \ell \cos \theta)$$

The Lagrangian can be simplified by adding a total derivative:

Let $F(\theta, t) = m\ell\dot{y}_s(t) \cos \theta + mg \int y_s(t) dt - \frac{1}{2}m \int \dot{y}_s^2(t) dt$, then

$$\frac{dF}{dt} = m\ell\ddot{y}_s(t) \cos \theta - m\ell\dot{y}_s(t) \sin \theta \dot{\theta} + mgy_s(t) - \frac{1}{2}m\dot{y}_s^2$$

and letting $L' = L + \frac{dF}{dt}$

$$L' = \frac{1}{2}m\ell^2\dot{\theta}^2 + m\ell(g + \ddot{y}_s(t)) \cos \theta$$

which is an easier Lagrangian to work with. In particular the explicit time dependence appears as a coefficient of the $\cos \theta$ term which results in parametric forcing.

Noether's Theorem and conserved quantities

We have already seen that conserved quantities result when the Lagrangian is not explicitly a function of one of the generalized coordinates. If say

$$\frac{\partial L}{\partial q_i} = 0 \quad \text{then, from the Euler-Lagrange equations,} \quad \frac{\partial L}{\partial \dot{q}_i} \quad \text{is a constant of the motion.}$$

In the spherical pendulum the axial momentum is conserved because the Lagrangian is not a function of ϕ . The fact that the Lagrangian is not a function of q_i implies an underlying symmetry in the system. For instance the spherical pendulum is symmetrical about the vertical axis. So it is the underlying symmetries of the system that imply the conserved quantities. Noether's theorem proves that the existence of conserved quantities in a system is closely linked to the symmetries of the system. **In fact she proved that for any continuous symmetry there is a conserved quantity.**

Consider a system undergoing a translation parametrised by s which does not change the Lagrangian and which is not time dependent. (Actually time dependence can be allowed.) The translated generalised coordinates will be denoted $\mathbf{q}_s$ where $\mathbf{q}_0 = \mathbf{q}$.

Now $\mathbf{q}$ satisfies Lagrange's equations

$$\frac{\partial L}{\partial q_j} - \frac{d}{dt} \left(\frac{\partial L}{\partial \dot{q}_j} \right) = 0. \quad (1 \leq j \leq n)$$

So that multiplying by $\left[\frac{\partial q_{sj}}{\partial s} \right]_{s=0}$ and summing over j gives

$$\begin{aligned} 0 &= \sum_{j=1}^n \frac{\partial L}{\partial q_j} \left[\frac{\partial q_{sj}}{\partial s} \right]_{s=0} - \sum_{j=1}^n \frac{d}{dt} \left(\frac{\partial L}{\partial \dot{q}_j} \right) \left[\frac{\partial q_{sj}}{\partial s} \right]_{s=0} \\ 0 &= \sum_{j=1}^n \left[\frac{\partial L}{\partial q_{sj}} \frac{\partial q_{sj}}{\partial s} \right]_{s=0} - \frac{d}{dt} \sum_{j=1}^n \left[\left(\frac{\partial L}{\partial \dot{q}_{sq}} \right) \frac{\partial q_{sj}}{\partial s} \right]_{s=0} + \sum_{j=1}^n \left[\frac{\partial L}{\partial \dot{q}_{sq}} \frac{\partial \dot{q}_{sq}}{\partial s} \right]_{s=0} \end{aligned}$$

Or rearranging

$$\frac{\partial L}{\partial s} = \frac{d}{dt} \sum_{j=1}^n \left[\left(\frac{\partial L}{\partial \dot{q}_{sq}} \right) \frac{\partial q_{sj}}{\partial s} \right]_{s=0}$$

But the Lagrangian is unchanged by the translation so $\frac{\partial L}{\partial s} = 0$.

This means that

$$\frac{d}{dt} \sum_{j=1}^n \frac{\partial L}{\partial \dot{q}_j} \left[\frac{\partial q_{sj}}{\partial s} \right]_{s=0} = 0$$

or

$$\sum_{j=1}^n \frac{\partial L}{\partial \dot{q}_j} \left[\frac{\partial q_{sj}}{\partial s} \right]_{s=0} \quad \text{is a conserved quantity}$$

Take the example of a particle in two dimensions where

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

Since the potential is a function of $r^2 = x^2 + y^2$ the rotation

$$\begin{pmatrix} x_s \\ y_s \end{pmatrix} = \begin{pmatrix} \cos s & -\sin s \\ \sin s & \cos s \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} \quad \text{leaves } L \text{ unchanged.}$$

To see this

$$\frac{\partial L}{\partial s} = m \left(\dot{x} \frac{\partial \dot{x}}{\partial s} + \dot{y} \frac{\partial \dot{y}}{\partial s} \right) - U' \left(2x \frac{\partial x}{\partial s} + 2y \frac{\partial y}{\partial s} \right)$$

$$\frac{\partial L}{\partial s} = 0 - U' (2x(-x_s \sin s + y_s \cos s) + 2y(-x_s \cos s - y_s \sin s)) = -U' (2x(y) + 2y(-x)) = 0$$

As in the theorem

$$\frac{\partial L}{\partial s} = \frac{\partial L}{\partial x} \frac{\partial x}{\partial s} + \frac{\partial L}{\partial y} \frac{\partial y}{\partial s} + \frac{\partial L}{\partial \dot{x}} \frac{\partial \dot{x}}{\partial s} + \frac{\partial L}{\partial \dot{y}} \frac{\partial \dot{y}}{\partial s}$$

Using Lagrange's equations

$$\frac{\partial L}{\partial s} = \frac{d}{dt} \left(\frac{\partial L}{\partial \dot{x}} \right) \frac{\partial x}{\partial s} + \frac{\partial L}{\partial \dot{x}} \frac{d}{dt} \left(\frac{\partial x}{\partial s} \right) + \frac{d}{dt} \left(\frac{\partial L}{\partial \dot{y}} \right) \frac{\partial y}{\partial s} + \frac{\partial L}{\partial \dot{y}} \frac{d}{dt} \left(\frac{\partial y}{\partial s} \right)$$

$$\frac{\partial L}{\partial s} = \frac{d}{dt} \left(\frac{\partial L}{\partial \dot{x}} \frac{\partial x}{\partial s} + \frac{\partial L}{\partial \dot{y}} \frac{\partial y}{\partial s} \right)$$

So

$$\frac{\partial L}{\partial s} = 0 \Rightarrow \frac{\partial L}{\partial \dot{x}} \frac{\partial x}{\partial s} + \frac{\partial L}{\partial \dot{y}} \frac{\partial y}{\partial s} \quad \text{is a conserved quantity}$$

Here

$$\frac{\partial L}{\partial \dot{x}} \frac{\partial x}{\partial s} + \frac{\partial L}{\partial \dot{y}} \frac{\partial y}{\partial s} = m(\dot{x}(-y) + \dot{y}x)$$

which is the angular momentum.