The Calculus of Variations

As we saw when we discussed path integrals, the amplitude

$$\langle \phi | \psi, T \rangle = \langle \phi | e^{-iTH/\hbar} | \psi \rangle = \langle \phi | e^{-iT\left(\frac{p^2}{2m} + V(x)\right)/\hbar} | \psi \rangle$$

$$= \int Dx(t)\, e^{iS[x]/\hbar} \langle \phi | x(T) \rangle \langle x(0) | \psi \rangle$$

where $S[x]$ is the classical action

$$S[x(\cdot)] = \int_0^T dt\, L(x, \dot{x}) = \int_0^T dt \left[\frac{m}{2} \dot{x}^2(t) - V(x(t)) \right].$$

Two paths that differ by $\delta x(t)$ may wash each other out unless the action S is stationary,

$0 = \delta S$, which means that $\delta S \propto \delta x^2$. This is the principle of least action.

In fact, much of classical physics follows from a choice of S and the rule $0 = \delta S$.

Example: (Note $\delta \dot{x} = \dot{x} + \dot{\delta x} - \dot{x} = d\,\delta x/dt$.)

$$\delta S = \int_0^T dt\, m \dot{x}\, \delta \dot{x} - V' \delta x + O(\delta x^2)$$

$$= \int_0^T dt - \delta x \left(m \ddot{x} + V' \right) + \left[m \dot{x}\, \delta x \right]_0^T,$$

since we dropped δx^2.

If the two paths $x(t)$ and $x(t) + \delta x(t)$ both go from $x(0)$ to $x(T)$, then

$$\delta x(0) = \delta x(T) = 0$$

and the boundary terms vanish. Then

$$\delta S = -\int_0^T dt \left(m\ddot{x} + V' \right) \delta x$$

So if $\delta S \propto \delta x^2$, ~~and~~ not $\delta \propto \delta x$, then

$$0 = \delta S = -\int_0^T dt \; (m\ddot{x} + V') \, \delta x$$

and since δx is arbitrary (but small), we get

$$m\ddot{x} + V' = 0 \quad \text{or} \quad m\ddot{x} = -V' \quad \text{or}$$

$$m\ddot{x} = F = ma = \frac{\partial V(x)}{\partial x}.$$

In books on classical mechanics, one often uses generalized coordinates $q_i(t)$ so that

$$S = \int_0^T dt \; L(q, \dot{q}, t),$$

in which q and $\dot{q}$ stand for $q_1 \cdots q_N$, etc.

Now the action S will be stationary if

$$0 = \delta S = \int_0^T dt \left(\frac{\partial L}{\partial q_i} \delta q_i + \frac{\partial L}{\partial \dot{q}_i} \delta \dot{q}_i \right).$$

Now

$$\delta \dot{q}_i = \dot{q}_i + \delta \dot{q}_i - \dot{q}_i = \frac{d}{dt} \delta q_i, \text{ so}$$

again integrating by parts, we have

$$\delta S = \int_0^T dt \; \delta q_i \left(\frac{\partial L}{\partial q_i} - \frac{d}{dt} \frac{\partial L}{\partial \dot{q}_i} \right) + \left[\frac{\partial L}{\partial \dot{q}_i} \delta q_i \right]_0^T .$$

If all the paths go from $q_i(0)$ to $q_i(T)$, then

$\delta q_i(0) = \delta q_i(T) = 0$ and we have

$$0 = \delta S \quad \text{if} \quad \frac{\partial L}{\partial q_i} - \frac{d}{dt} \frac{\partial L}{\partial \dot{q}_i} = 0 .$$

The canonical momentum p_i is

$$p_i = \frac{\partial L}{\partial \dot{q}_i} \quad \text{and so}$$

Lagrange's equations imply $\dot{p}_i = \dfrac{\partial L}{\partial q_i}$.

Usually the Lagrangian $L(q, \dot{q})$ does not involve t explicitly. In this case, one may define a hamiltonian H that is conserved:

$$H = \sum_{i=1}^{N} p_i \dot{q}_i - L$$

To see that $\dot{H}$ vanishes, just take its time derivative

$$\dot{H} = \sum_{i=1}^{N} \left(\dot{p}_i \dot{q}_i + p_i \ddot{q}_i - \frac{\partial L}{\partial q_i} \dot{q}_i - \frac{\partial L}{\partial \dot{q}_i} \ddot{q}_i \right)$$

But $p_i = \dfrac{\partial L}{\partial \dot{q}_i}$ and $\dot{p}_i = \dfrac{\partial L}{\partial q_i}$, so $\dot{H} = 0$.

Now suppose $\mathcal{L}(\phi, \phi_{,j})$ is a Lagrange density that depends on the fields $\phi_1, \phi_2 \cdots \phi_N$ and their derivatives

$$\phi_{i,j} = \frac{\partial \phi_i}{\partial x_j} .$$

Assume that $\delta \phi_i = 0$ when any argument $x_K \to \pm \infty$, so we can drop all surface terms. Then

$$L = \int d^3x \, \mathcal{L} \quad \text{and} \quad S = \int dt \, L = \int d^4x \, \mathcal{L} .$$

The requirement that δS be quadratic or higher in $\delta \phi$ gives

$$0 = \delta S = \int d^4x \; \frac{\partial \mathcal{L}}{\partial \phi_i} \delta \phi_i + \frac{\partial \mathcal{L}}{\partial \phi_{i,j}} \delta \phi_{i,j}$$

Now $\quad \delta\phi_{i,j} = (\phi_i + \delta\phi_i)_{,j} - \phi_{i,j} = (\delta\phi_i)_{,j}$

where $G_{,j} = \dfrac{\partial G}{\partial x_j}$, as before. So

$$0 = \delta S = \int d^4x \;\; \delta\phi_i \left(\frac{\partial \mathcal{L}}{\partial \phi_i} - \left(\frac{\partial \mathcal{L}}{\partial \phi_{i,j}} \right)_{,j} \right) + \underset{0}{\overset{\|}{\text{S.T.}}}$$

whence the field equations

$$0 = \frac{\partial \mathcal{L}}{\partial \phi_i} - \frac{\partial}{\partial x_j} \left(\frac{\partial \mathcal{L}}{\partial \phi_{i,j}} \right).$$

In this way, one does field theory.

Lagrange Multipliers

Suppose one wants to find x and y that maximize $f(x,y)$ subject to the constraint $g(x,y) = c$, a constant. Set

$$H(x,y,\lambda) = f(x,y) + \lambda(g(x,y) - c)$$

and find the x, y, & λ that maximize H. Then

$$\left.\begin{aligned} 0 = \frac{\partial H}{\partial x} = H_x &= f_x + \lambda g_x = 0 \\ 0 = H_y &= f_y + \lambda g_y = 0 \\ 0 = H_\lambda &= g - c = 0. \end{aligned}\right\}$$

Solve these three eqs, for x, y, and λ.

Why does this work? Well, one could solve for the curve $y(x)$ that keeps

$$g(x, y(x)) = c.$$

Then one can maximize $f(x, y(x))$ by setting its derivative equal to zero:

$0 = f_x + y' f_y$. To find y', one sets

$0 = g_x + y' g_y$, which gives $y' = -\frac{1}{g_y} g_x$.

So

$$0 = f_x + y' f_y = f_x - \frac{1}{g_y} g_x f_y \quad \text{or}$$

$$0 = f_x - \frac{f_y}{g_y} g_x \qquad \text{ie} \quad \lambda = -\frac{f_y}{g_y}$$

and

$$0 = f_y + \frac{1}{y'} f_x$$

$$0 = f_y - \frac{g_y}{g_x} f_x = f_y - \frac{f_x}{g_x} g_y \quad \text{ie} \quad \lambda = -\frac{f_x}{g_x}.$$

So

$$0 = f_x - \frac{f_y}{g_y} g_x$$

$$0 = f_y - \frac{f_x}{g_x} g_y$$

and the two equations for λ are the same because

$$0 = f_x - \frac{g_x}{g_y} f_y \quad \text{which means} \quad \frac{f_x}{g_x} = \frac{f_y}{g_y} = -\lambda.$$

Suppose $\rho = \sum \rho_n |n\rangle\langle n|$ is a density operator. Then $\langle F \rangle = \mathrm{tr}(\rho F)$

and $1 = \langle 1 \rangle = \operatorname{tr} \rho$. And $\langle H \rangle = \operatorname{tr} \rho H$.

Now $S = -k \operatorname{tr}(\rho \log \rho)$. So let's maximize S

subject to the conditions $1 = \operatorname{tr} \rho$ and $E = \langle H \rangle$.

So we maximize

$$Z(\rho, \lambda, \mu) = S + \lambda(E - \langle H \rangle) + \mu(1 - \langle 1 \rangle)$$

$$= -k \operatorname{tr}(\rho \log \rho) + \lambda(E - \operatorname{tr} H\rho) + \mu(1 - \operatorname{tr} \rho)$$

We suppose $\langle n | m' \rangle = \delta_{mm'}$

$$H|n\rangle = E_n |n\rangle. \quad \text{So}$$

$$Z(\rho, \lambda, \mu) = -k \sum \rho_n \log \rho_n + \lambda\left(E - \sum \rho_n E_n\right) + \mu\left(1 - \sum \rho_n\right)$$

$$0 = \frac{\partial Z}{\partial \rho_n} = -k \log \rho_n - \lambda E_n - \mu, \quad \text{so}$$

$$\log \rho_n = (-\lambda E_n - \mu)/k$$

$$\rho_n = e^{(-\lambda E_n - \mu)/k}$$

Choose μ, by setting $\rho_n = \dfrac{e^{-\frac{\lambda E_n}{k}}}{\sum_n e^{-\lambda E_n / k}}$.

Choose $\lambda = \dfrac{1}{T}$

by the rule $\sum \rho_n E_n = E$.

Then

$$\rho_n = \frac{e^{-\frac{E_n}{kT}}}{\sum_n e^{-E_n/kT}}$$

is the quantum density operator that maximizes entropy for a fixed mean value E of the energy while conserving probability

$$\mathrm{tr}\,\rho = 1.$$

Chaos

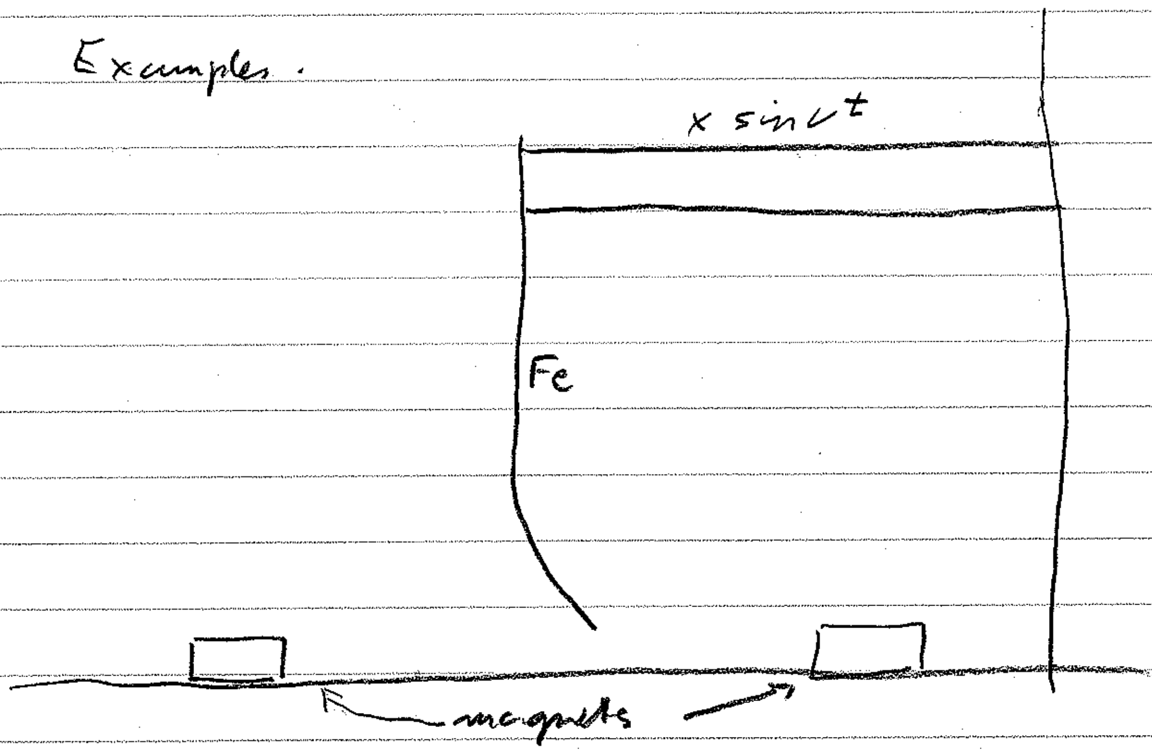
Henri Poincaré (~1900) studied the three-body problem and found very complicated (chaotic) orbits.

There seem to be four kinds of classical motion

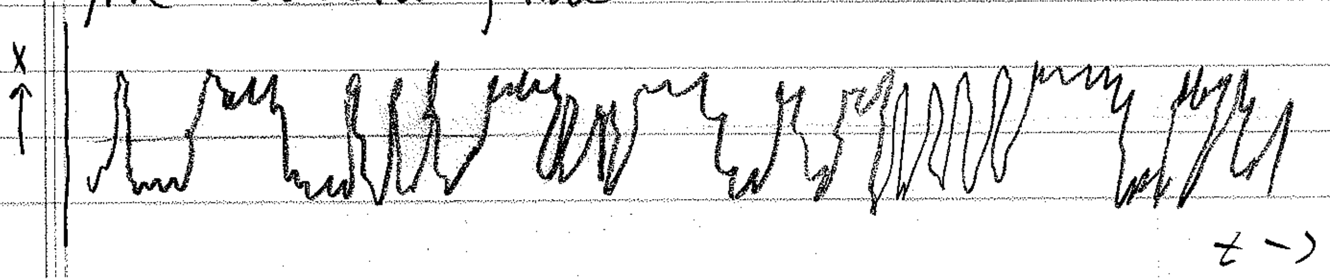
1) periodic
2) steady (or damped motion that stops)
3) quasiperiodic (mixture of periodic motions, ω_i)
4) chaotic

for a system after a transient period.

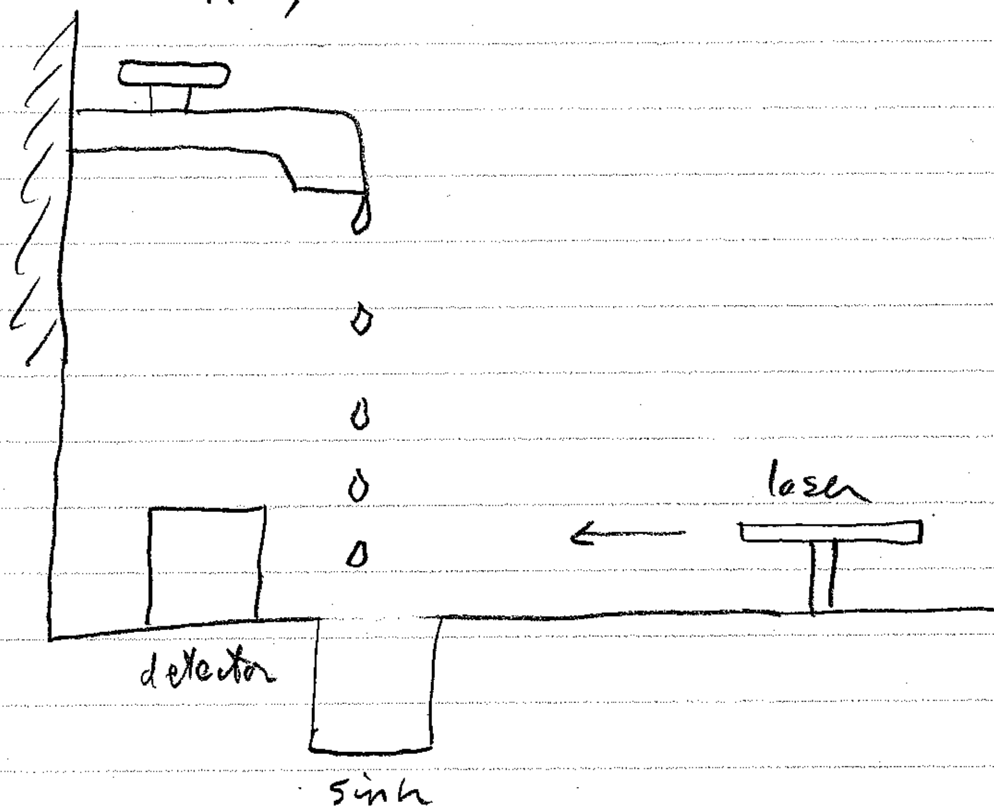
Examples.



$\ddot{x} + \nu\dot{x} + x^3 - x = g\sin t$ Exp. & theory give something like



Dripping faucet



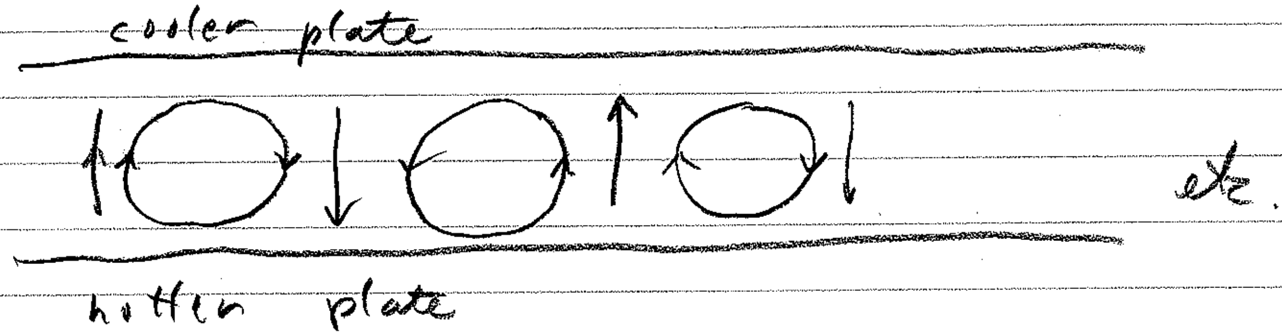
Data are t_1, t_2, t_3 ...

At low flow rate, $\Delta t_n = t_{n+1} - t_n$ is constant, all Δt_n are equal.

At a slightly higher rate, the drops come with gaps that alternate $\Delta t_a, \Delta t_b, \Delta t_a, \Delta t_b, \ldots$ so that $\Delta t_{n+2} = \Delta t_n$. This is a period-two sequence.

At still higher flow rates, no regularity is apparent.

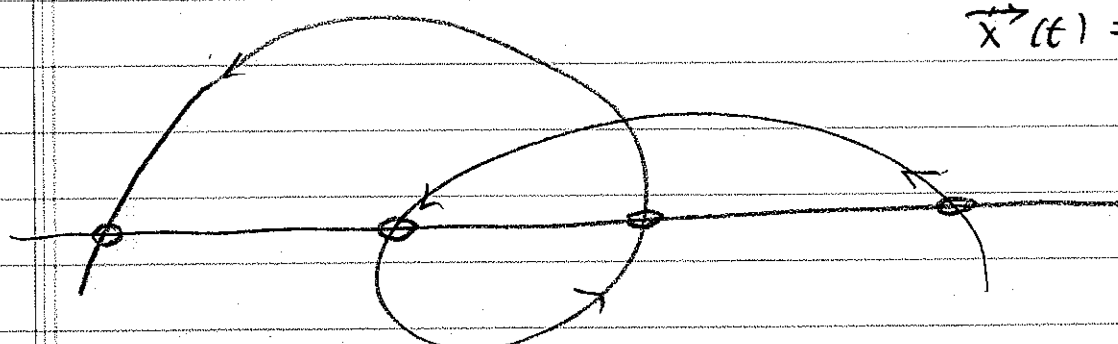
Chaotic Rayleigh - Benard convection occurs when a fluid is placed in a gravitational field between two plates that are kept at constant temperatures with the lower plate hotter by Δt above the chaotic threshold. For lower Δt, the motion is steady convective cellular flow



Dynamical Systems

$$\dot{x}_i = F_i(x) \quad \text{or} \quad \dot{\vec{x}} = \vec{F}(\vec{x}),\ \text{ie}$$

$$\dot{\vec{x}}(t) = \vec{F}(\vec{x}(t))$$



The crossings of a suitably oriented plane give rise to a map

$$\vec{x}_{n+1} = \vec{M}(x_n)$$

in ~~one~~ fewer dimensions.

In the system

$$\dot{\vec{x}} = \vec{F}(\vec{x})$$

chaos can occur only if the dimension N of the vector $\vec{x}$ exceeds 2

$$N \geq 3.$$

For the invertible map

$$x_{n+1} = M(x_n) \Rightarrow x_n = M^{-1}(x_{n+1})$$

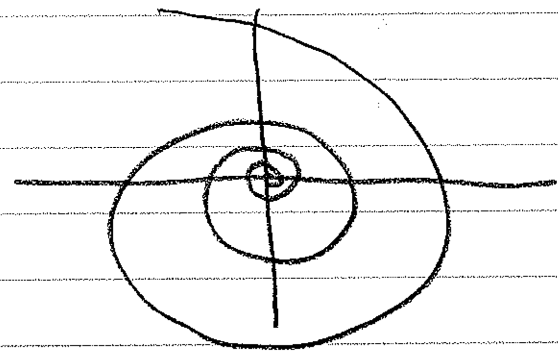
chaos occurs only if $N \geq 2$.

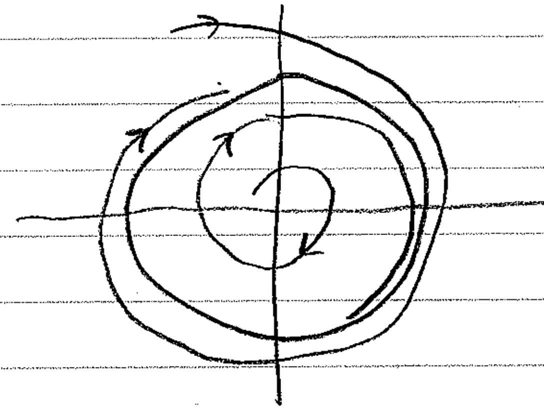
If the map is not invertible, then chaos can occur even if $N = 1$. An example is

$$x_{n+1} = r\, x_n(x_n - 1)$$

which is not invertible and does exhibit chaos in increasingly striking forms as r exceeds a number slightly greater than $r_m = 3.57$. By $r = 4$, the map is totally chaotic.

Attractors





Here $x_1 = x_2 = 0$ is an attractor.

Here the circle is an attractor called a <u>limit cycle</u>.

The limit cycle occurs in the van der Pol equation

$$\ddot{y} + (y^2 - \eta)\dot{y} + \omega^2 y = 0$$

which may be written as the first-order system

$$x_1 = \dot{y} \qquad x_2 = y$$

$$\dot{x}_1 = -\omega^2 x_2 - (x_2^2 - \eta) x_1$$

$$\dot{x}_2 = x_1$$

The van der Pol equation was introduced in the 1920's to describe a vacuum-tube oscillator circuit.

Fractals

Fractal sets don't have dimensions that are natural numbers. To compute their dimensions one needs a definition of dimension.

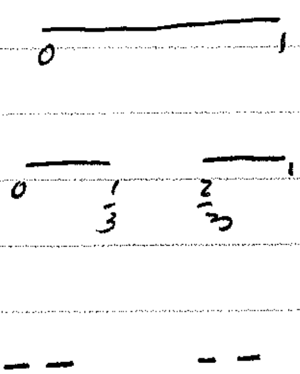
The box-counting dimension is as follows: Cover the set with line segments, squares, cubes, etc., of edge length ϵ. Count how many you need as $\epsilon \to 0$. Call the number of boxes $N(\epsilon)$. Then

$$D_0 = \lim_{\epsilon \to 0} \frac{\ln N(\epsilon)}{\ln (1/\epsilon)},$$

Cantor set: 0

1

2



$\epsilon_n = \left(\frac{1}{3}\right)^n$ need $N(\epsilon) = 2^n$ boxes.

So

$$D_0 = \lim_{n \to \infty} \frac{\ln 2^n}{\ln 3^n} = \lim \frac{\ln 2}{\ln 3} \simeq 0.63.$$

Attractors of fractal dimension are <u>strange</u>.