Computational Physics

PHYS4150/8150 (6 credits)

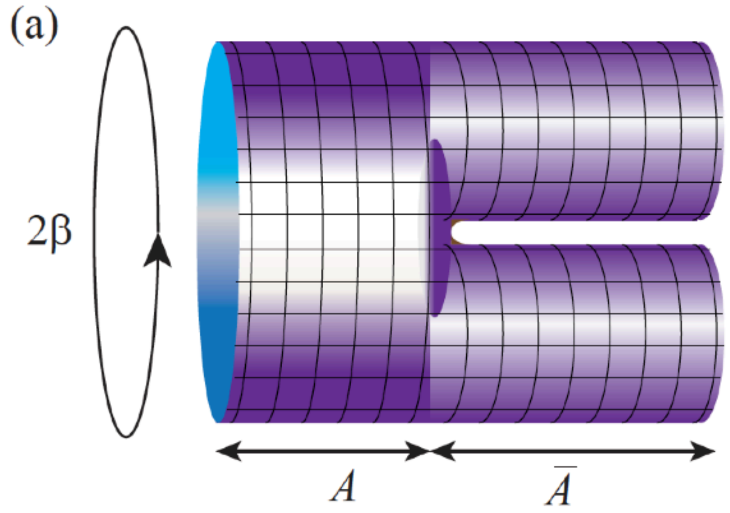
Place: KKL 201

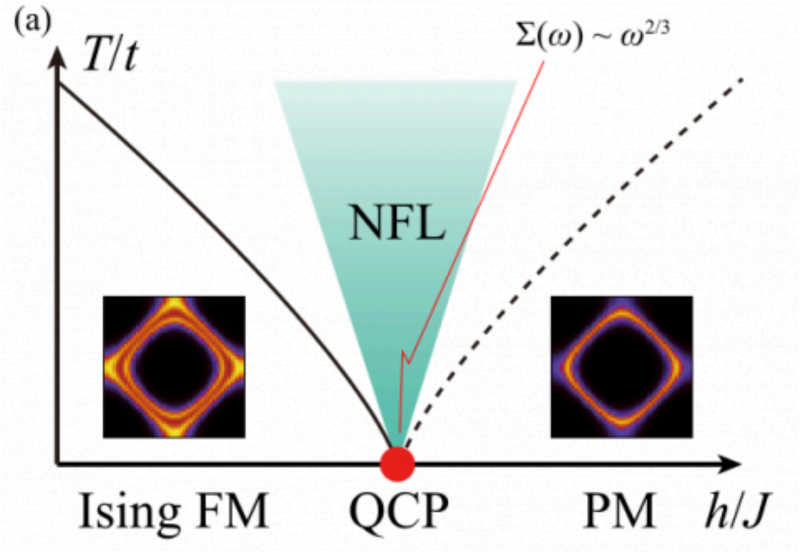
Time : Mon 17:30-18:20
Thu 16:30-17:20; 17:30-18:20

https://quantummc.xyz/teaching/hku-phys4150-8150-computational-physics-2024/

Teacher: Zi Yang Meng (zymeng@hku.hk)

Tutor: Tim-Lok Chau (Justin) (justintlchau@connect.hku.hk)
Min Long (minlo@connect.hku.hk)

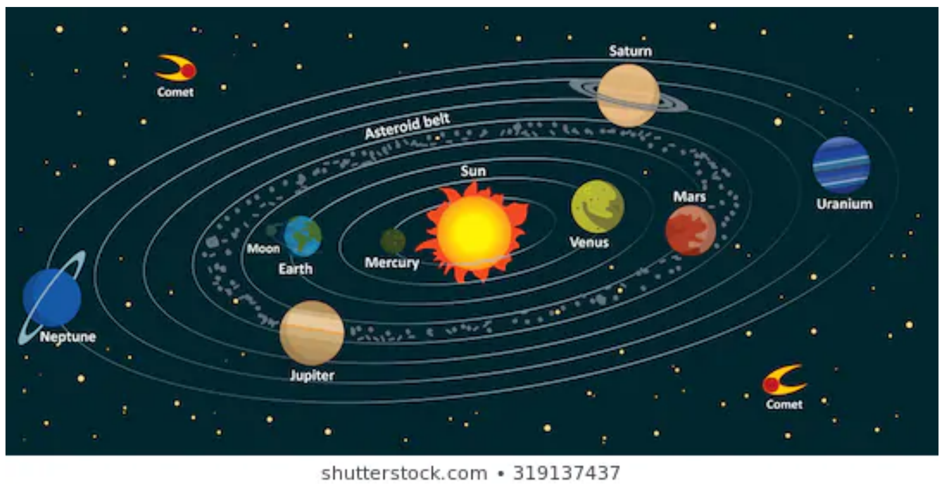




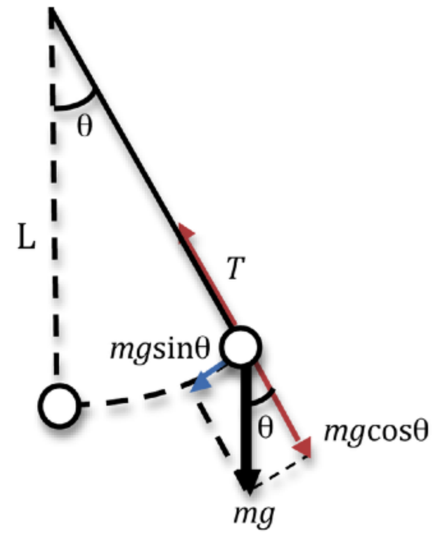
Content

Differential equations

- Initial value problems: time-dependent equations with given initial conditions



Solar system



Pendulum

浮世绘，葛饰北斋，神奈川冲浪里

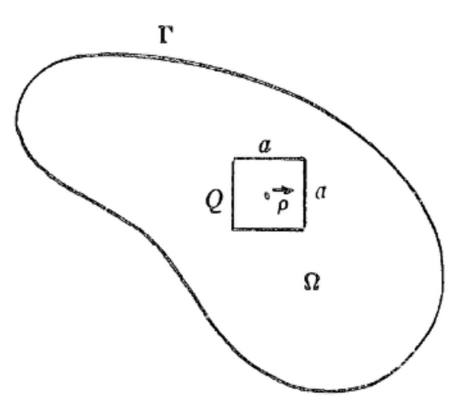
- Boundary value problems: differential equations with specific boundary values

CAN ONE HEAR THE SHAPE OF A DRUM?

MARK KAC, The Rockefeller University, New York

To George Eugene Uhlenbeck on the occasion of his sixty-fifth birthday

- Am. Math. Mon. 73, 1 (1966)



Eigenvalues of Dirichlet problem for Laplacian

$$\tfrac{1}{2}\nabla^2 U + \lambda U = 0 \text{ in } \Omega,$$
$$U = 0 \text{ on } \Gamma.$$

Length of circumference

$$\sum_{n=1}^{\infty} e^{-\lambda_n t} \sim \frac{|\Omega|}{2\pi t} - \frac{L}{4}\frac{1}{\sqrt{2\pi t}} + \frac{1}{6}$$

Number of holes

$$(1-r)\frac{1}{6}$$

- Eigenvalue problems

Classical equation of motion

Differential equations

$$\dot{\vec{v}}_i(t) = \vec{a}_i(\vec{x}_0(t), \cdots, \vec{x}_{N-1}(t), \vec{v}_0(t), \cdots, \vec{v}_{N-1}(t), t)$$

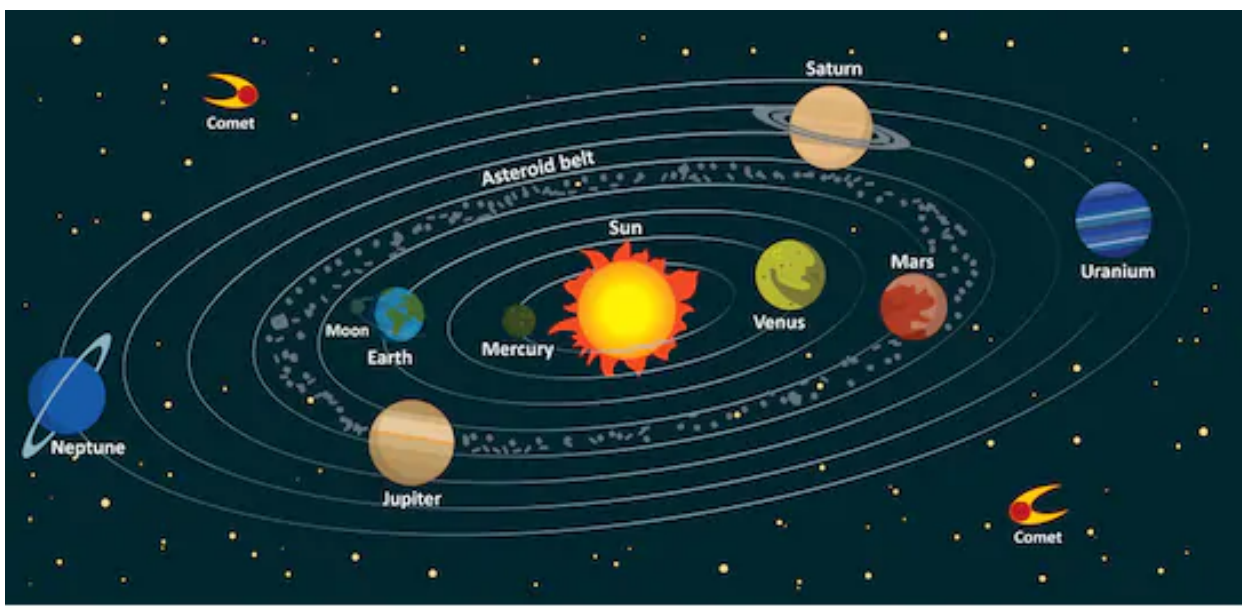
State of dynamical system

$$\dot{\vec{x}}_i(t) = \vec{v}_i(t) \qquad i = 0, 1, \cdots, N-1$$

Gravitation (such as solar system)

$$\vec{a}_i(\vec{x}_0(t), \cdots, \vec{x}_{N-1}(t)) = G \sum_{j \neq i} \frac{m_j}{|\vec{x}_j(t) - \vec{x}_i(t)|^3} [\vec{x}_j(t) - \vec{x}_i(t)]$$

G Gravitational constant



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Discretization

$$t = t_0, t_1, t_2, \cdots \qquad \tau = t_{n+1} - t_n$$

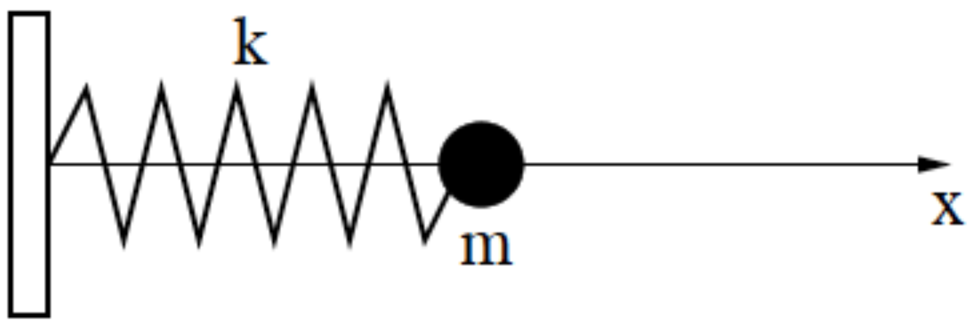
$$\vec{x}(t) = \begin{pmatrix} \vec{x}_0(t) \\ \vec{x}_1(t) \\ \vdots \\ \vec{x}_{N-1}(t) \end{pmatrix} \qquad \vec{v}(t) = \begin{pmatrix} \vec{v}_0(t) \\ \vec{v}_1(t) \\ \vdots \\ \vec{v}_{N-1}(t) \end{pmatrix}$$

$$\dot{\vec{v}}(t) = \vec{a}(\vec{x}(t), \vec{v}(t), t)$$

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

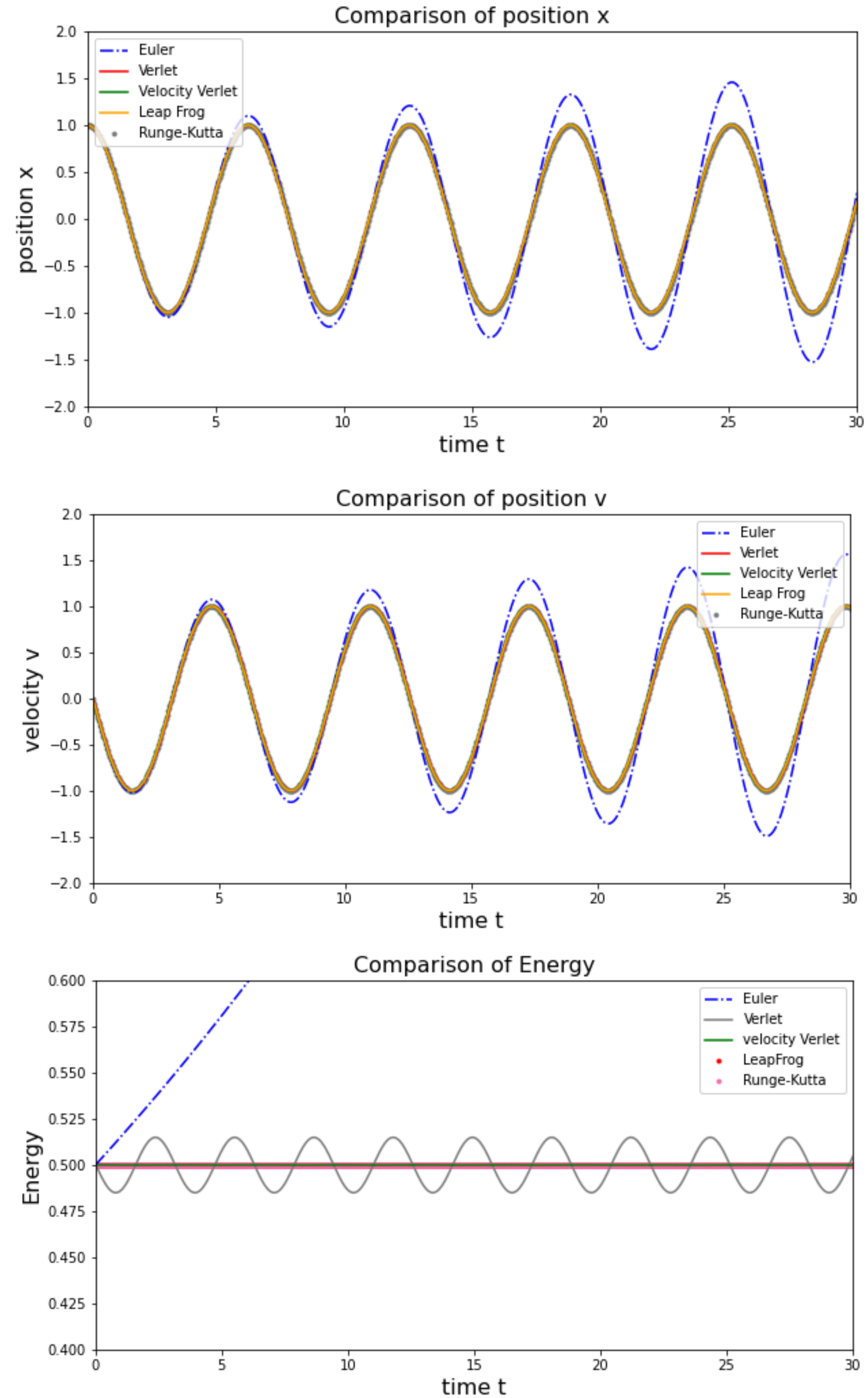
Classical equation of motion

Harmonic Oscillator



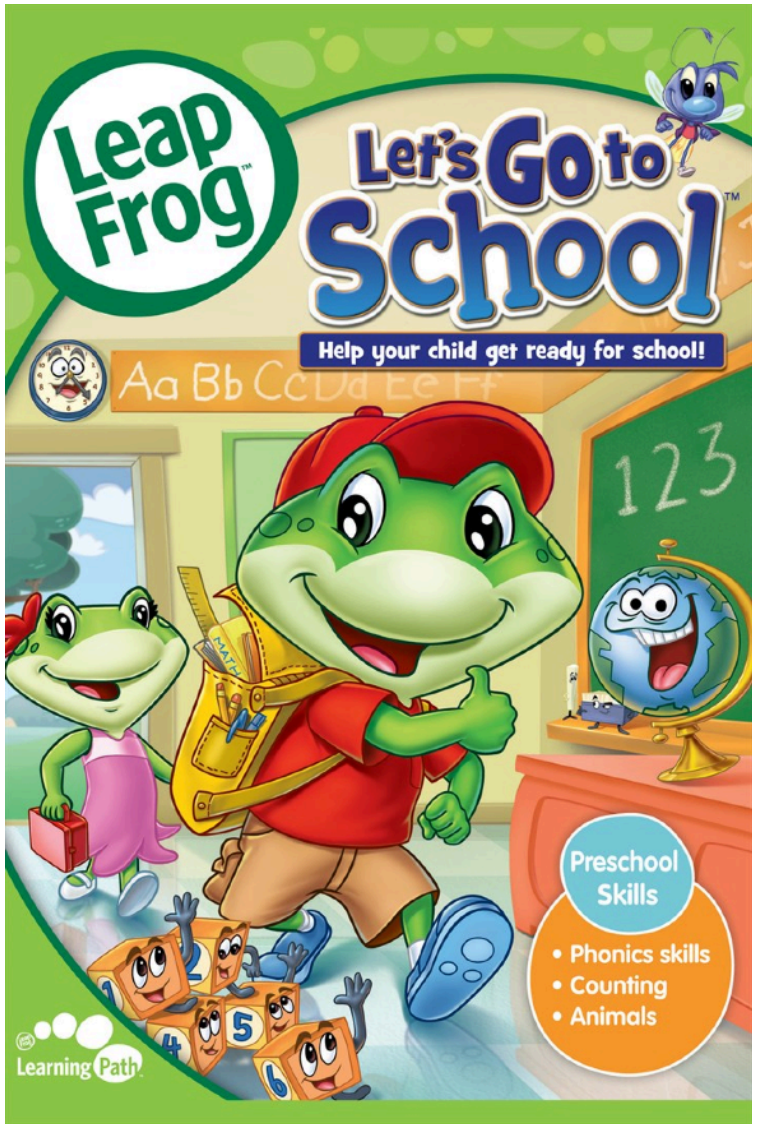
$$\vec{a}(t) = \dot{\vec{v}}(t) = -\frac{k}{m}x(t)$$

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



Initial value problem

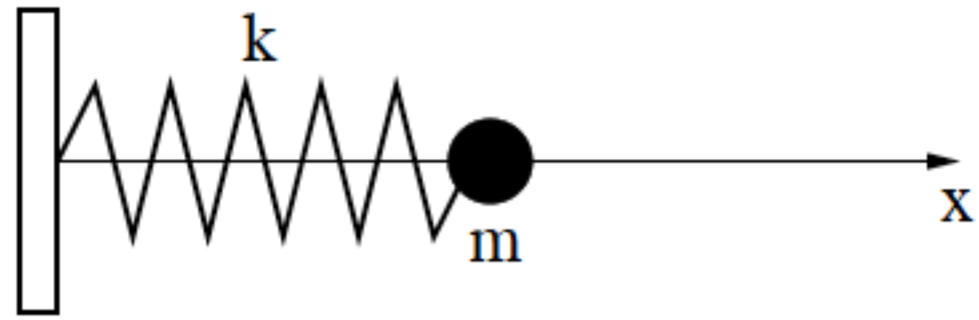
- Euler (tau^2)
- Verlet (tau^4, time-reversal)
- Velocity Verlet (variant of Verlet 1)
- Leap-frog (variant of Verlet 2, less roundoff error)
- Runge-Kutta (tau^5, workhorse)



LeapFrog Enterprises, Inc. is the leader in innovative solutions that encourage a child's curiosity and love of learning throughout their early developmental journey.

Classical equation of motion

Harmonic Oscillator

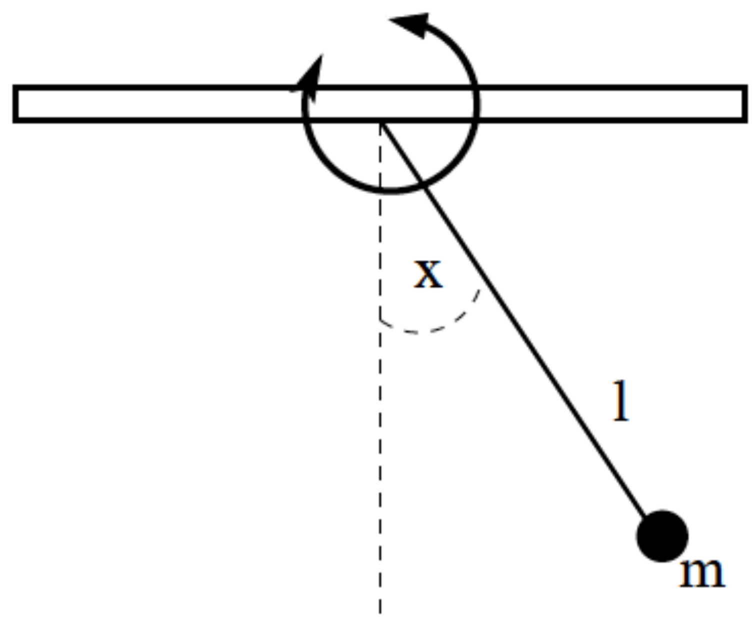


$$\dot{v}(t) = -\frac{k}{m}x$$

$$\dot{x}(t) = v$$

Driven Pendulum

Soliton solution



$$\gamma = 0 \quad \Omega = 0$$

goes back to harmonic oscillator at small x

$$g = 9.81 m/s^2$$

γ friction coefficient Stoke’s friction

Q strength of periodic driving force

Ω driving frequency

$$\dot{v}(t) = -\frac{g}{l}\sin(x) - \gamma\dot{x} + Q\sin(\Omega t)$$

$$\dot{x}(t) = v$$

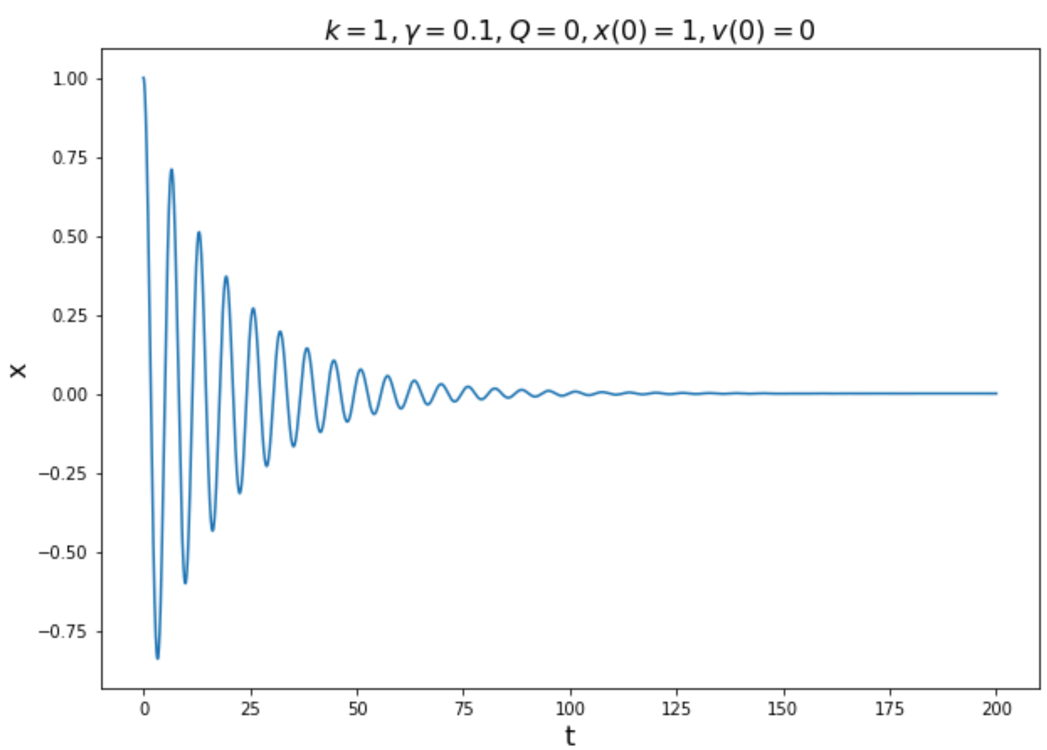
Many interesting videos https://www.youtube.com/watch?v=_TSp6KkMbP4

$$\ddot{x} = -k\sin(x) - \gamma\dot{x} + Q\sin(\Omega t) \qquad k = g/l = 1$$

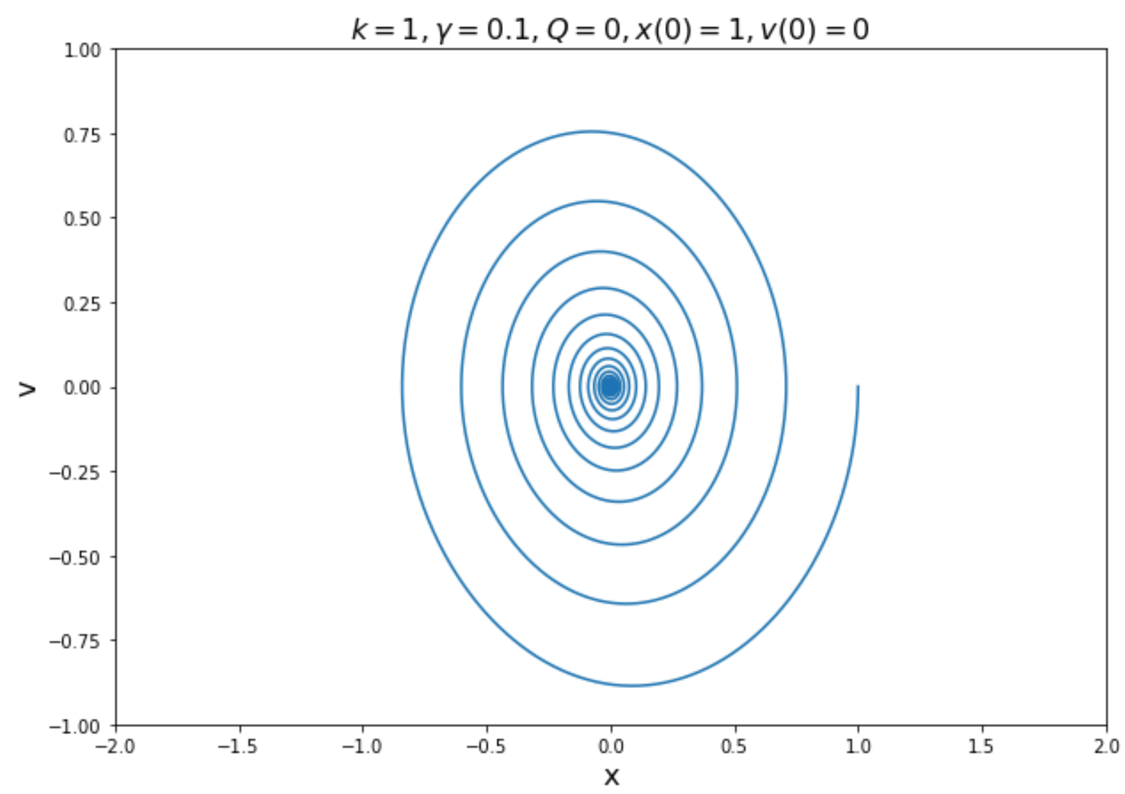
$\gamma \neq 0$ and $Q \neq 0$ no analytical solution $\qquad x \in [-\pi, \pi]$

$\gamma \neq 0$ and $Q = 0$

With friction only, damping



In phase space, attractor



$\gamma \neq 0$ and $Q \neq 0$

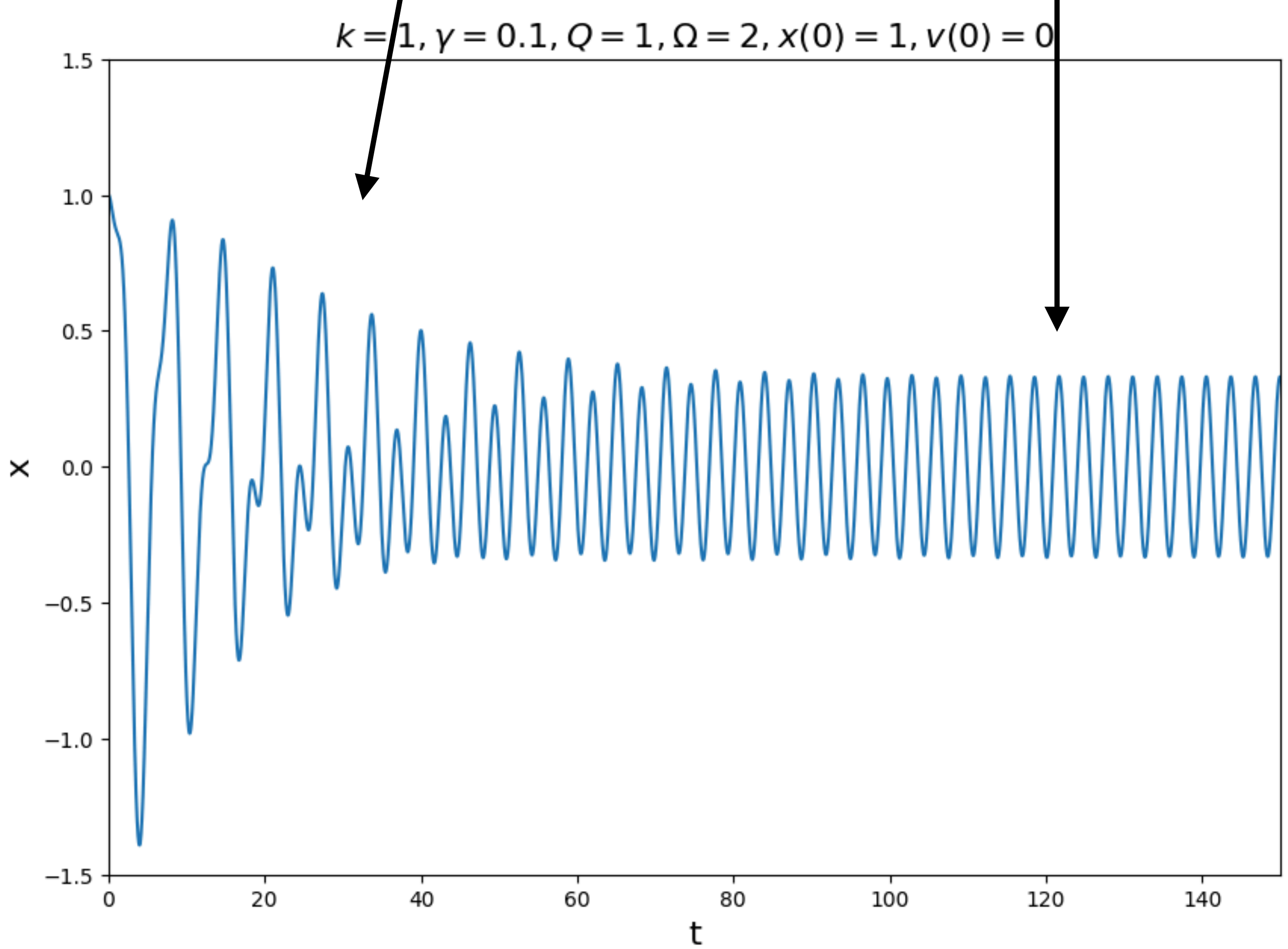
The original period $T = 2\pi\sqrt{\frac{l}{g}} = 2\pi\sqrt{\frac{m}{k}} = 2\pi$

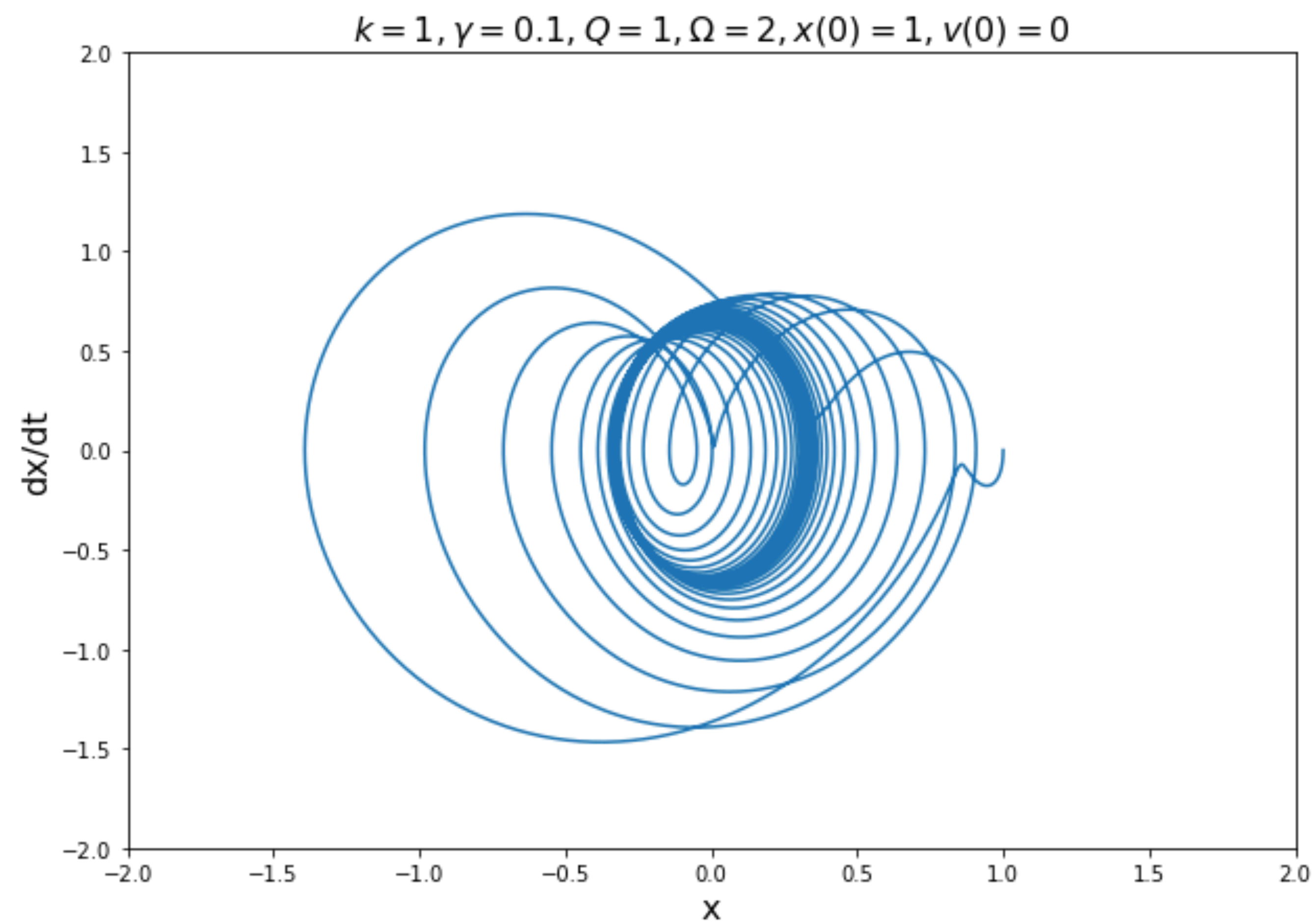
Initial damping and transient behaviour

In phase space, cyclic attractor

Driving force with frequency $\Omega = 2$

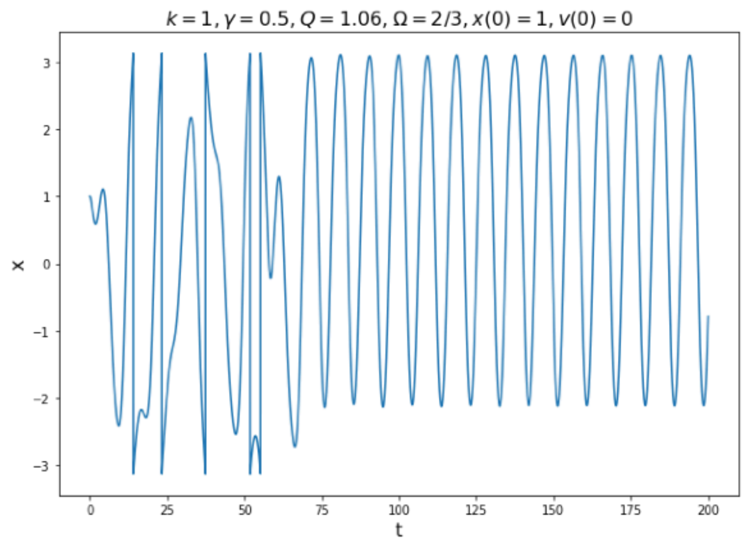
Period $T_\Omega = \frac{2\pi}{\Omega}$

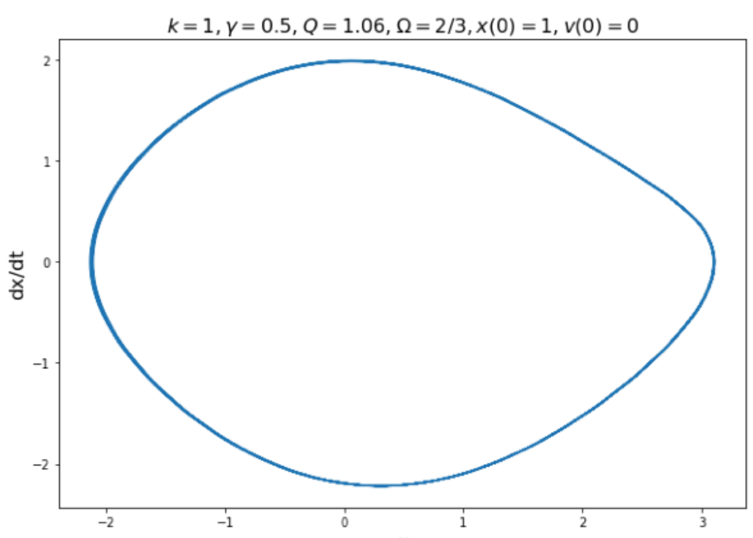




Asymmetric attractor
Spontaneous breaking of reflection symmetry

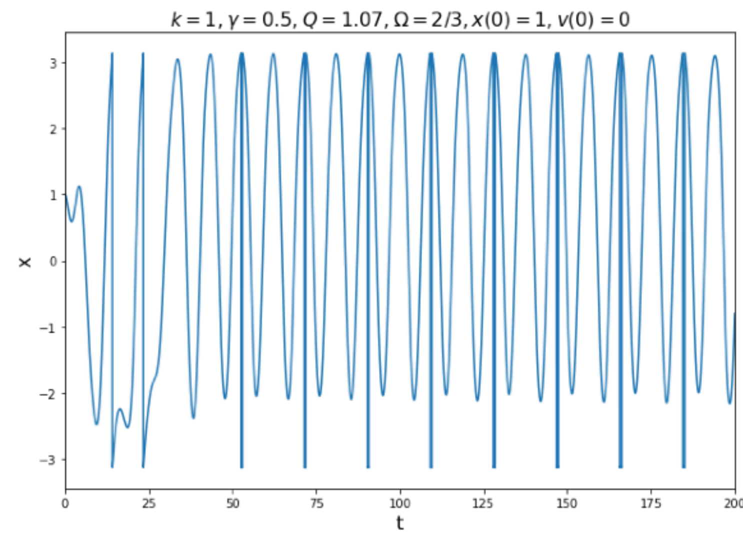
$(x, v) \neq (-x, -v) \quad Q = 1.06, \quad T = T_\Omega$

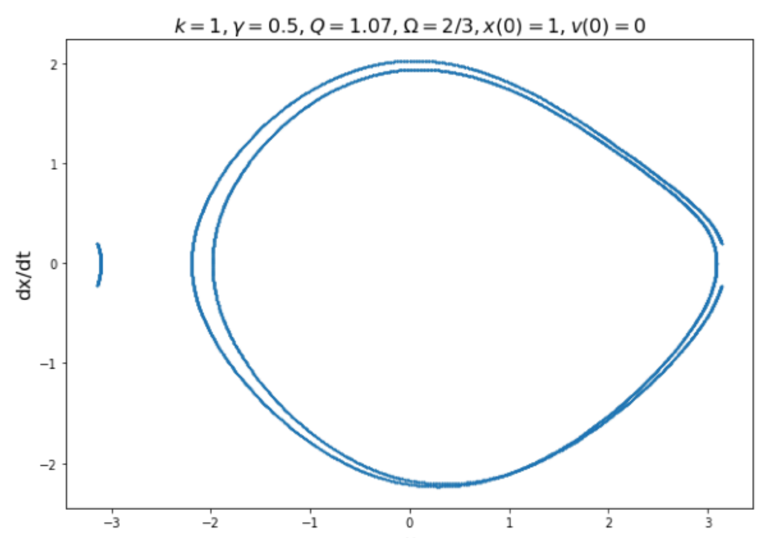




Period doubling

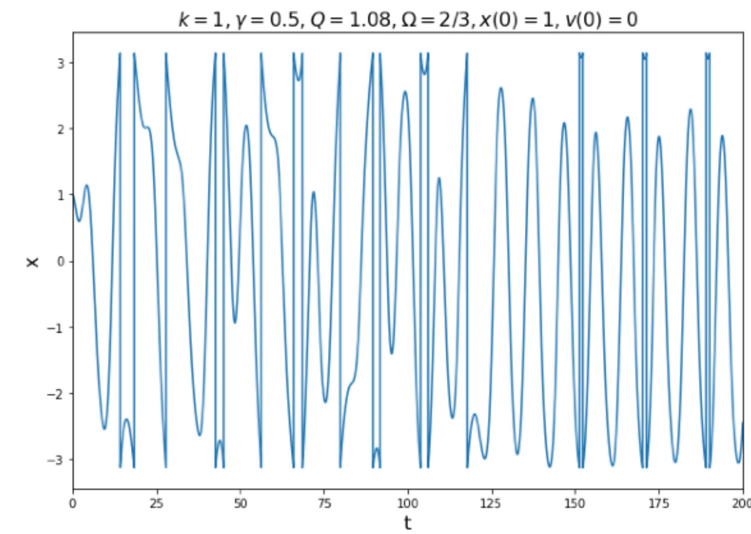
$Q = 1.07, \quad T = 2T_\Omega$

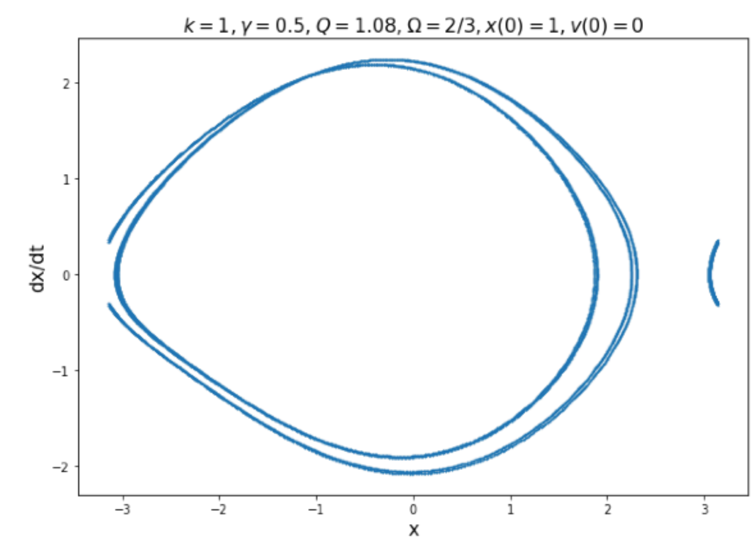




Further period doubling

$Q = 1.08, \quad T = 4T_\Omega$

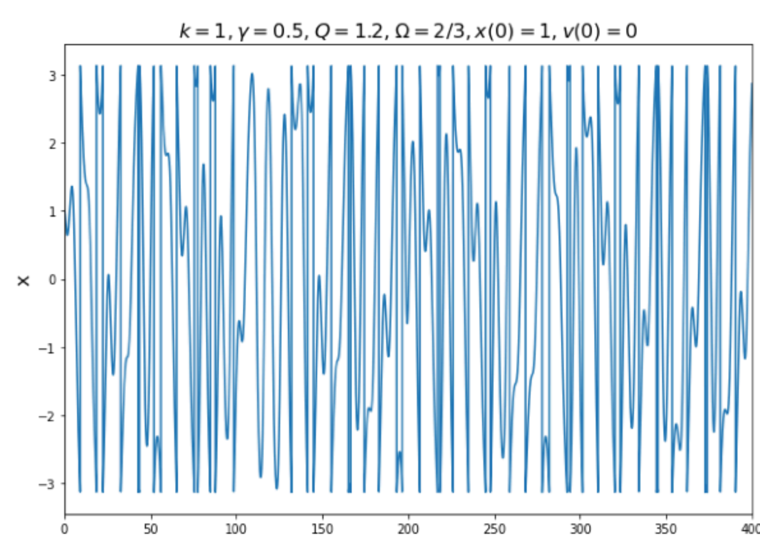


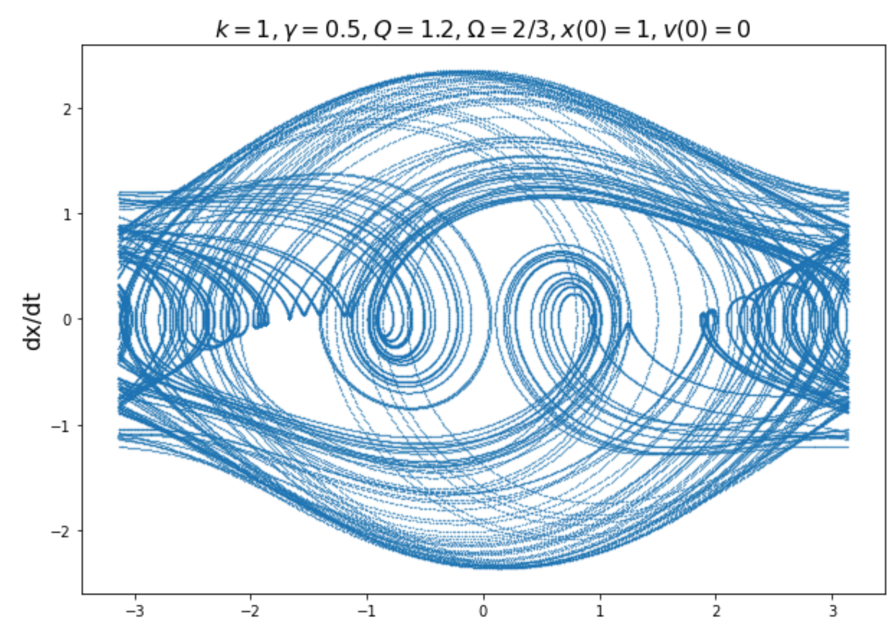


Chaotic attractor

$Q = 1.2$

The motion never closes, the attractor fills a finite region of the phase space





Chaos theory

https://en.wikipedia.org/wiki/Chaos_theory

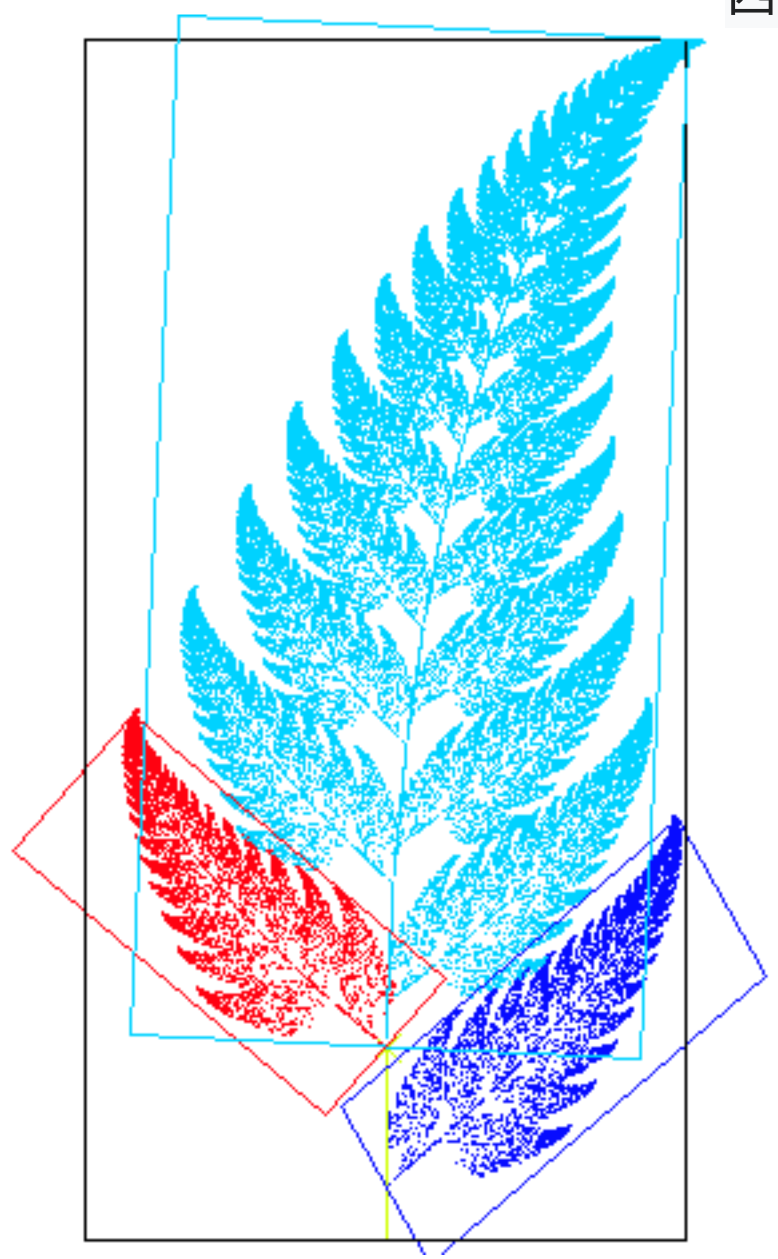
https://en.wikipedia.org/wiki/Chaos_theory#/media/File:Double-compound-pendulum.gif

Butterfly effect

Self-similarity

fractals

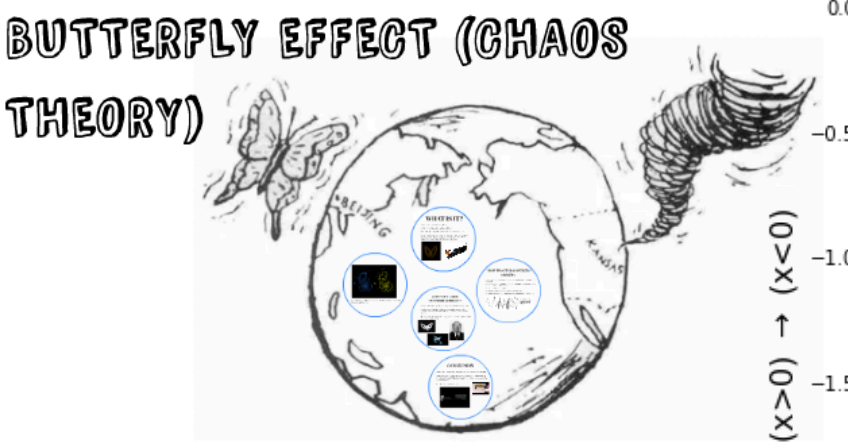
Self-organization

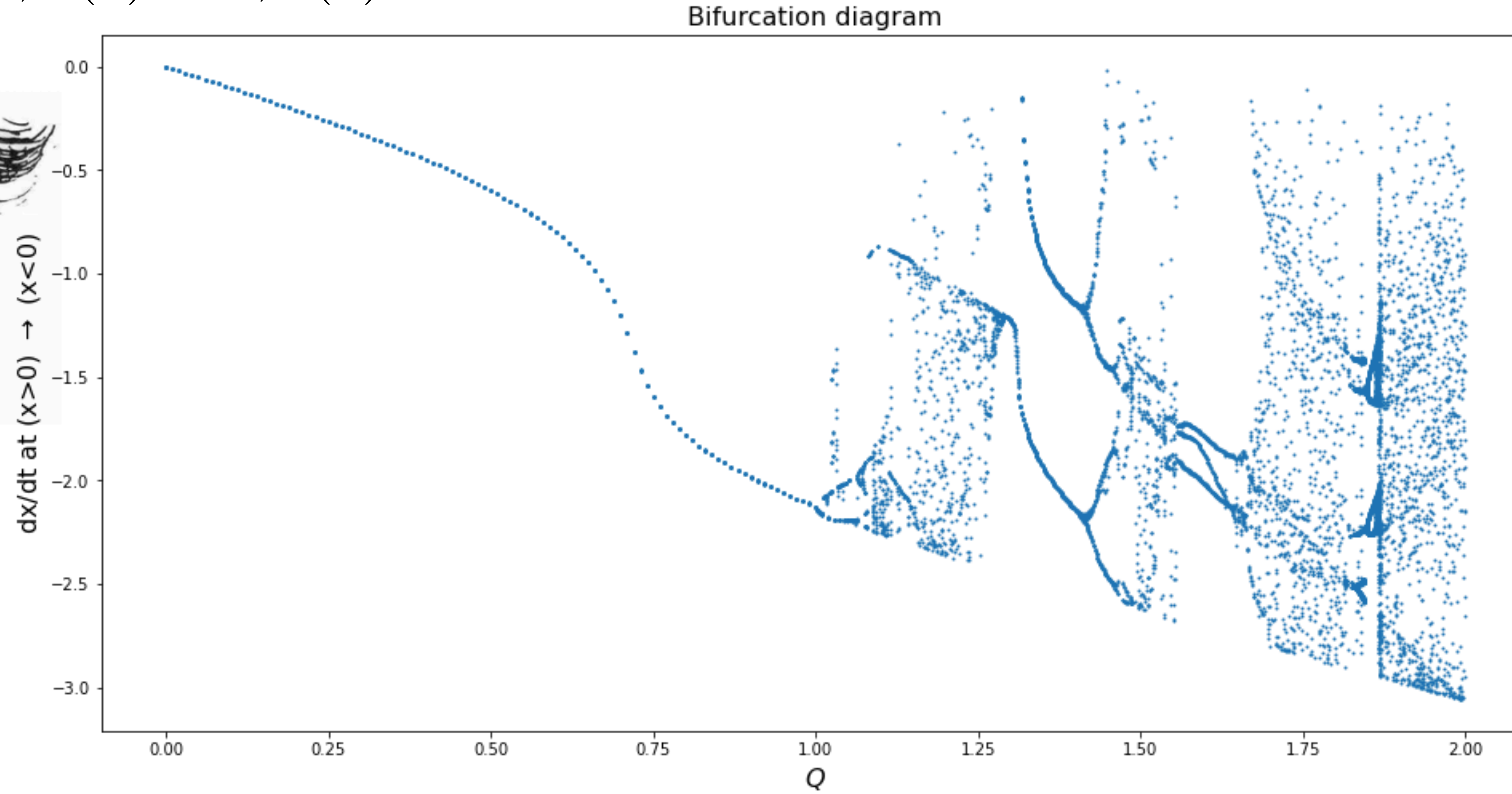


Romanesco broccoli
西兰花

Hausdorff dimensionality
Poincare section
Stroboscopic sampling

$$k = 1, \gamma = 0.5, \Omega = 2/3, x(0) = 1, v(0) = 0$$





Record the velocity as x passes 0 from above

Periodic motion, discrete set of period nT_Ω

Chaotic motion, many distinct values

Hausdorff dimensionality
Poincare section
Stroboscopic sampling

Many interesting videos https://www.myphysicslab.com/pendulum/chaotic-pendulum-en.html

Spectral Analysis and Power Spectrum

$$x(t) \qquad t_i = i \cdot \tau : i = 0,1,\cdots,N-1, \quad \tau = \frac{T}{N-1}$$

$$g(\omega) \qquad \omega_k = 2\pi k/(N\tau) : k = 0,1,\cdots,N-1, \quad \Delta\omega = 2\pi/(N\tau)$$

$$g(\omega_k) = \sum_{i=0}^{N-1} e^{-i\,\omega_k \cdot t_i}\, x_i = \sum_{i=0}^{N-1} e^{-i\frac{2\pi k}{N\tau} i\tau}\, x_i = \sum_{i=0}^{N-1} (W_N)^{ik}\, x_i \qquad W_N = e^{-i2\pi/N}$$

$$g_k = \sum_{i=0}^{N-1} (W_N)^{ik}\, x_i, \quad k = 0,1,\cdots,N-1$$

Starting from N time points, we have N frequencies

$$x_i = \frac{1}{N}\sum_{k=0}^{N-1} (W_N^*)^{ki}\, g_k, \quad i = 0,1,\cdots,N-1$$

$$= \frac{1}{N}\sum_{k=0}^{N-1}\sum_{j=0}^{N-1} (W_N^*)^{ki}(W_N)^{jk}\, x_j = \sum_{j=0}^{N} \Big(\frac{1}{N}\sum_{k=0}^{N-1} e^{-i\,2\pi k(i-j)/N}\Big) x_j = \sum_{j=0}^{N-1} \delta_{i,j}\, x_j = x_i$$

Direct Fourier Transformation: computational complexity $O(N^2)$

Fast Fourier Transformation: computational complexity $O(N \log_2 N)$

Chap.12.

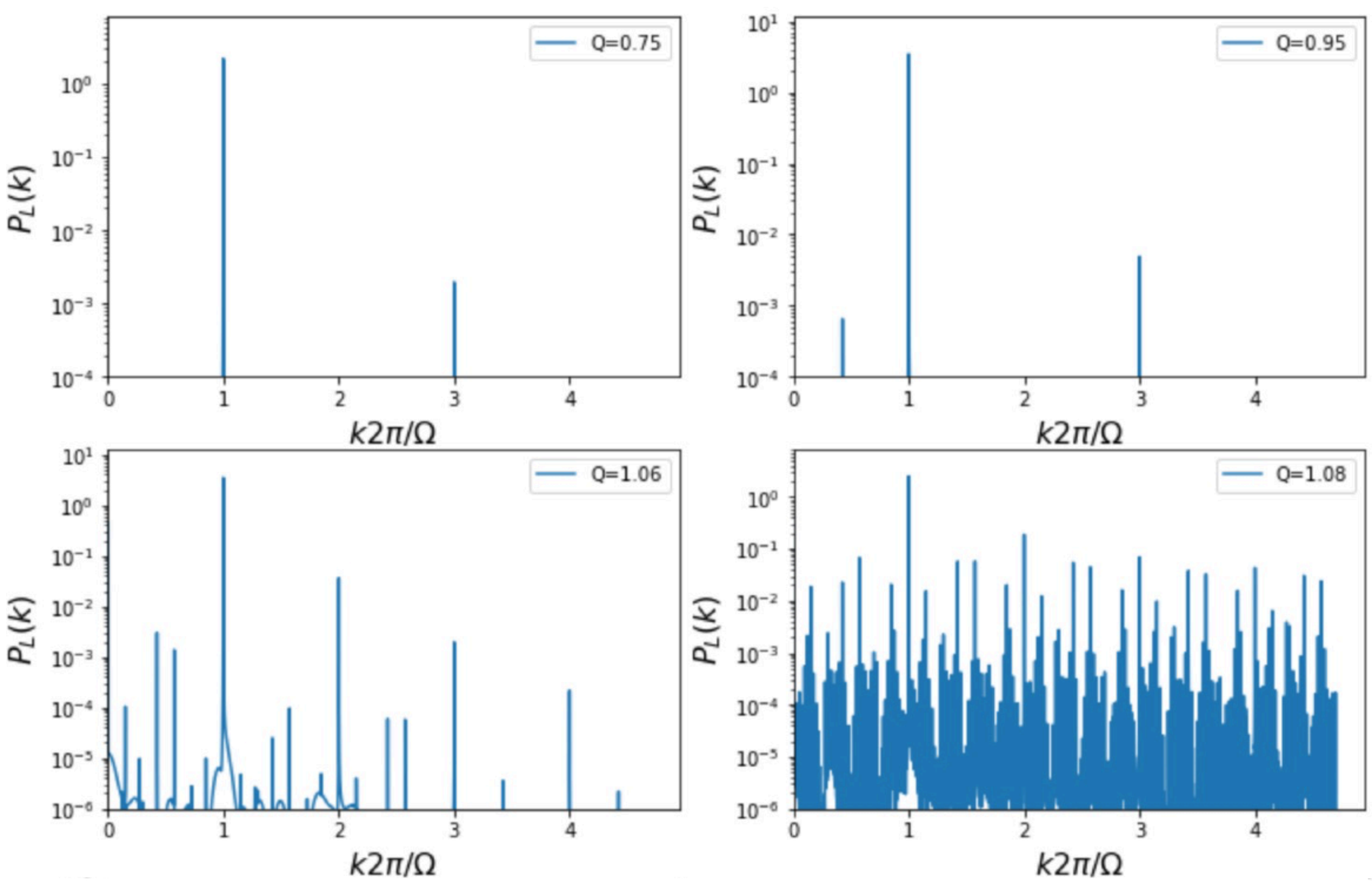
Power spectrum

space <—> momentum
time <—> frequency

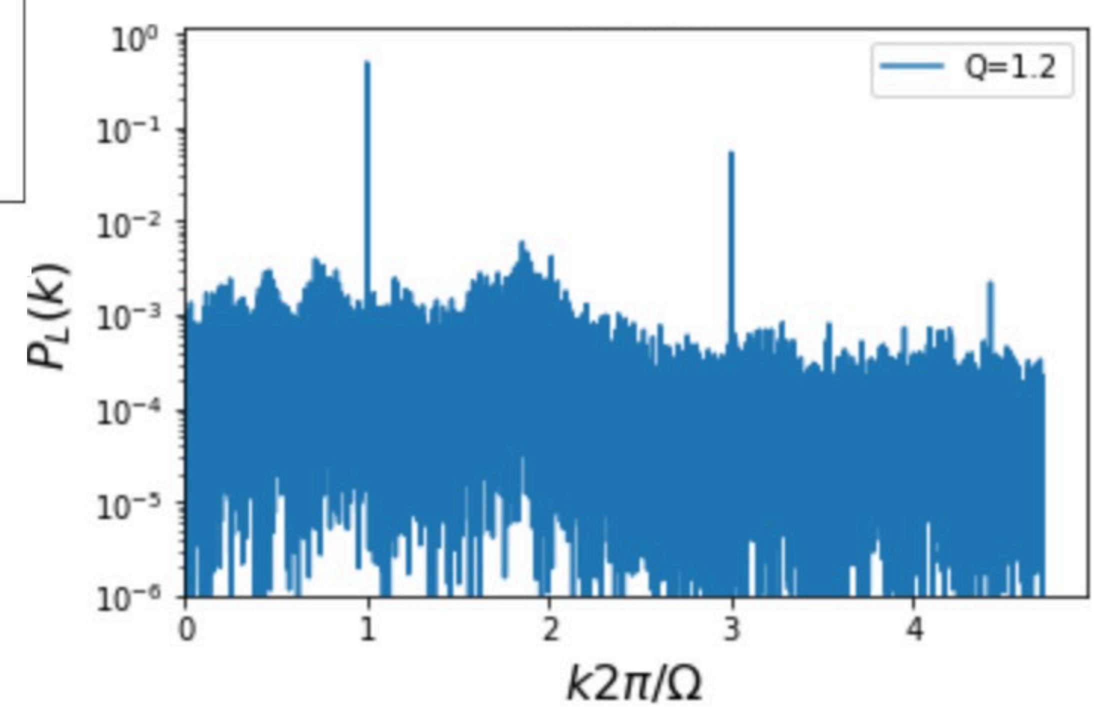
$$P(0) = \frac{1}{N^2} |g_0|^2$$

$$P(k) = \frac{1}{N^2} \left[|g_k|^2 + |g_{N-k}|^2 \right], \quad k = 1,2,\cdots,\frac{N}{2} - 1$$

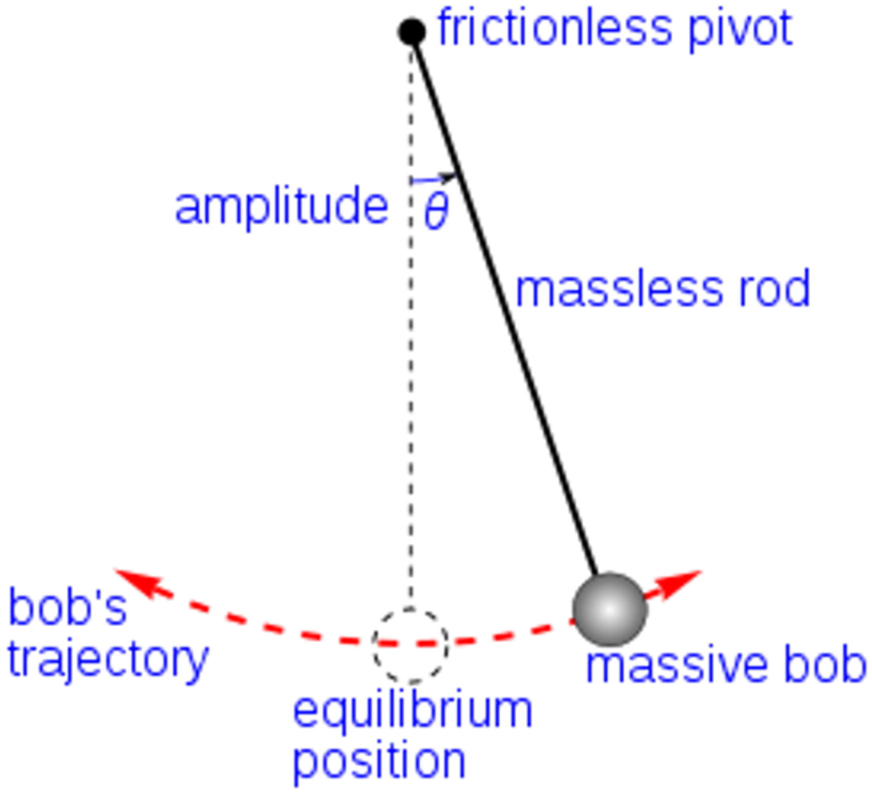
$$P(\frac{N}{2}) = \frac{1}{N^2} |g_{\frac{N}{2}}|^2$$ assume N is even

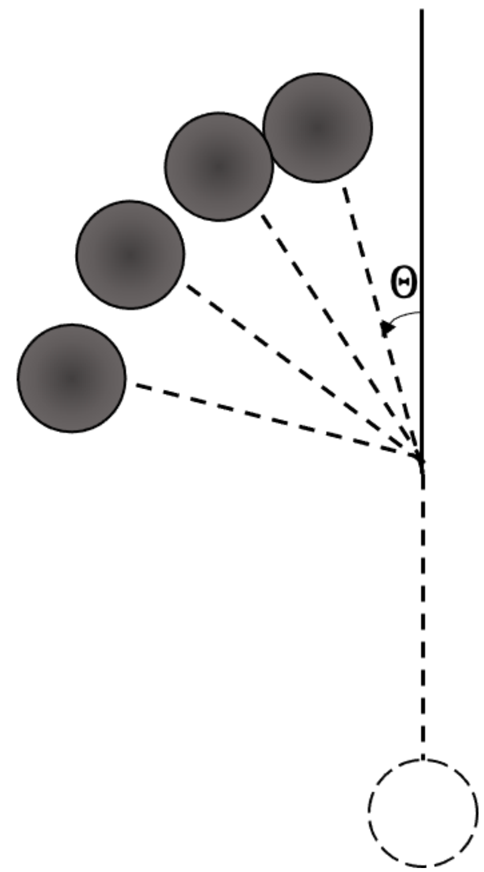


$$T = \frac{2\pi}{\Omega}$$



Soliton in pendulum



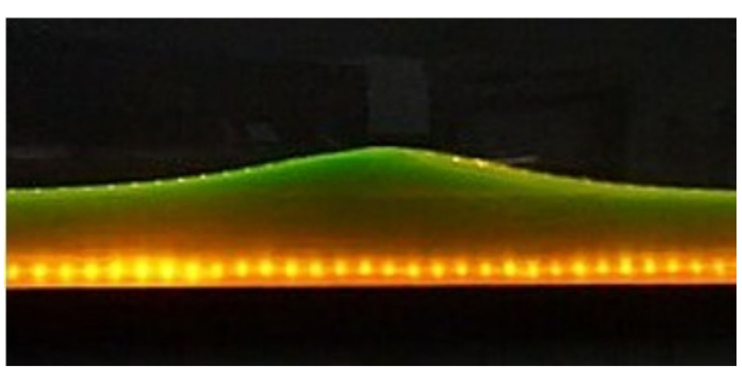


$$\theta = \theta + \pi$$

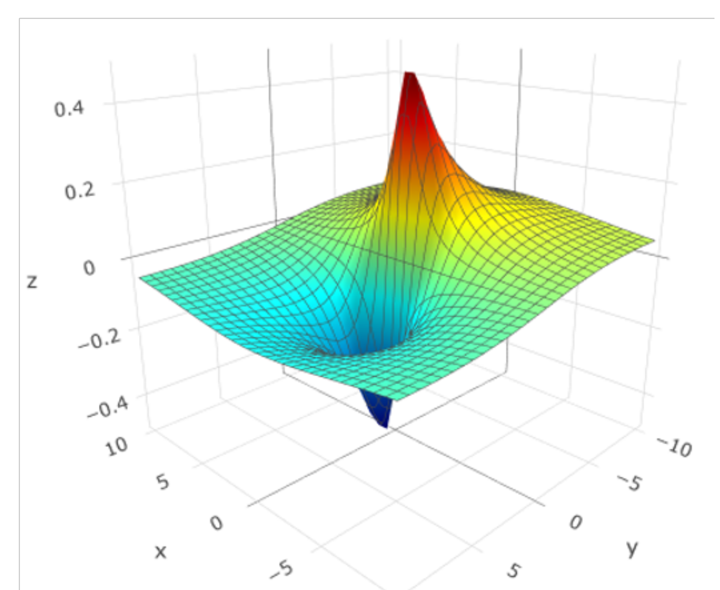
$$\ddot{\theta} = \frac{g}{l} \sin(\theta)$$

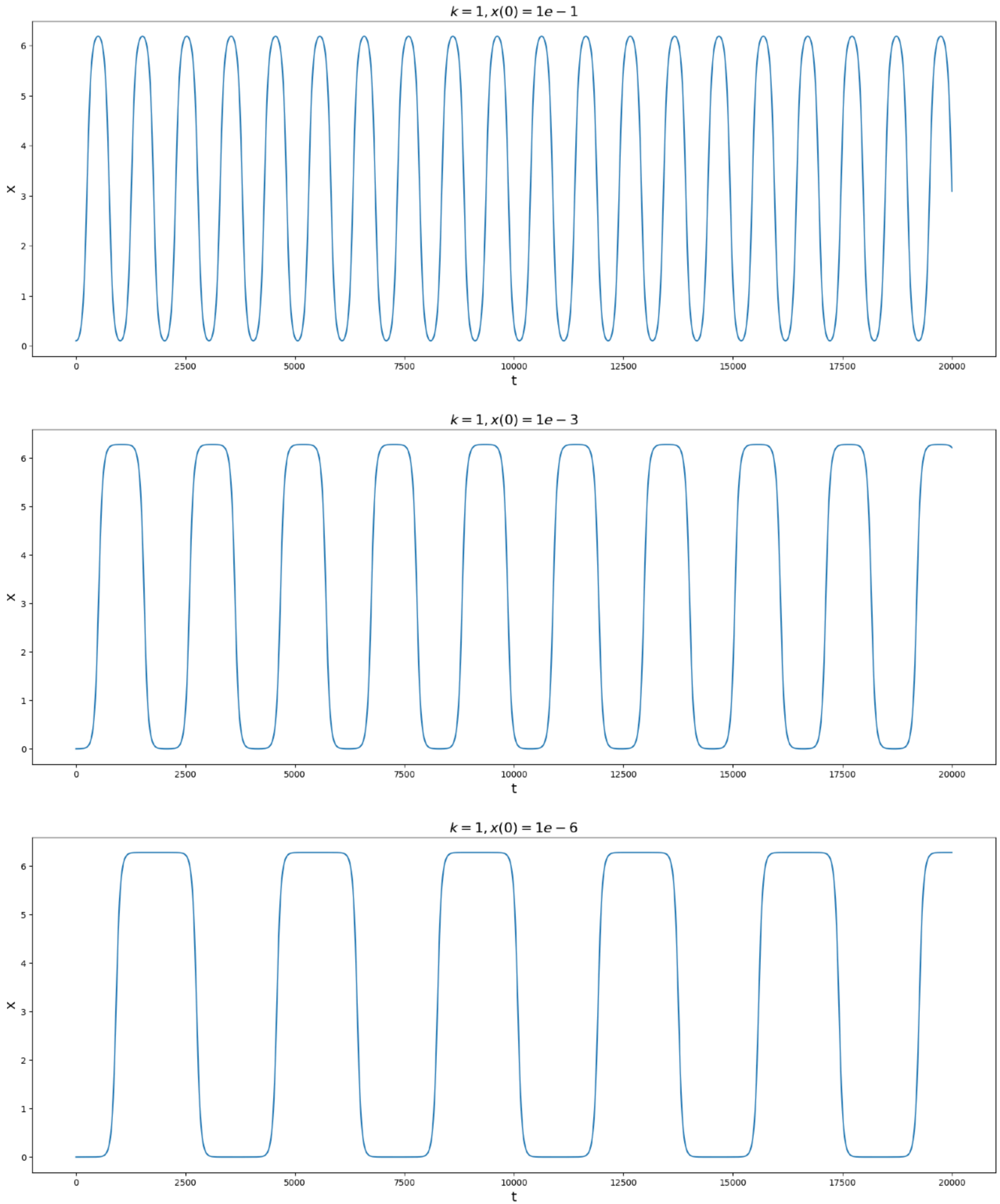
The ball will spend most of its time on the peak while rapidly go through the other region. Showing a well localized excitation at temporal space — Soliton or Instanton.

Classics soliton : water wave



BPST instanton: solution of equation of motion of SU(2) Yang-Mills theory in Euclidean space-time with winding-number 1. Meaning it describe the transition between two topologically different vaccum.





$k = 1, x(0) = 1e-1$
x
t
$k = 1, x(0) = 1e-3$
x
t
$k = 1, x(0) = 1e-6$
x
t