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Computational Physics I
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11.1. Lorenz System

It is a standard assumption in physics, that small effects which one typically neglects during the modeling of a system have a negligible impact on the final results. During a study of a model for the climate, Ed Lorenz discovered what became known as the *butterfly effect*: small differences in initial conditions can accumulate to give large differences later on.

The model which Lorenz studied consists of three differential equations:

$$\dot{x} = \sigma(y - x) \qquad \dot{y} = rx - y - xz \qquad \dot{z} = xy - bz \tag{1}$$

with parameters $\sigma = 10$ and $b = 8/3$ and r positive. It represents a caricature of convection in the atmosphere, with x the amplitude of a convection role, y the corresponding modulation in the temperature and z the change in the mean temperature profile. The system has three fixed points, and they are unstable when $r > 24.74...$.

Solve the equations of motion and follow the time evolution for $r = 28$ for a long time. What do you observe?

11.2 ODEs with periodic coefficients

A differential equation $\ddot{x} = -f(t)x$ with time periodic coefficients $f(t+T) = f(t)$ belong to the class of Hill's differential equations. With the specific form $f(t) = a + q\cos 2t$ the differential equation is known as Mathieu equation. For $q = 0$ and $a > 0$, the motion is periodic, for $a < 0$ the solutions grow exponentially. When q is non-zero, the periodicity of the force does not imply that the motion itself is periodic, but that the solution after a period can be expressed as a linear superposition of the fundamental solutions: The first fundamental solution $\vec{x}_1(t)$ solves the equations with initial conditions $x_1 = 1$ and $\dot{x}_1 = 0$, the second $\vec{x}_2(t)$ with initial conditions $x_2 = 0$ and $\dot{x}_2 = 1$. Every solution can be expressed as a linear combination of the two. Let $\vec{x}(t) = c_1\vec{x}_1(t) + c_2\vec{x}_2(t)$ with $c_1 = x$, $c_2 = \dot{x}$. After one period, one has

$$x(t+T) = a_{11}x(t) + a_{12}\dot{x}(t) \tag{2}$$
$$\dot{x}(t+T) = a_{21}x(t) + a_{22}\dot{x}(t) \tag{3}$$

where the coefficients $a_{1i} = x_i(T)$ and $a_{2i} = \dot{x}_i(T)$ form a 2×2 matrix of determinant 1. The trace of the matrix hence determines whether the solutions oscillate ($|tr| < 2$) or whether they grow exponentially in time ($|tr| > 2$).
Determine for the Mathieu equation the trace as a function of a and q and find the values in a for $q = 0.2$ for which the motion is stable (oscillates).

11.3 Quantum eigenvalues using shooting method

Determine eigenfunctions and eigenvalues for an harmonic oscillator by solving a boundary problem with $\psi(L) = 0$ together with the conditions $\psi(0) = 1$ and $\psi'(0) = 0$ for the symmetric wave functions and $\psi'(0) = 1$ and $\psi(0) = 0$ for the antisymmetric ones.
How far out do you have to go with L so that the first two eigenvalues are accurate to 10^{-5}?
How large do you have to choose L so that the 10th eigenvalue is reproduced with a relative accuracy of 10^{-5}?

Now replace the harmonic potential with a Lennard-Jones potential of depth V_0 at $x = 1$ and determine the eigenvalues for the case $mV_0/\hbar^2 = 5$.