3.3: Newtonian Mechanics

Introduction goes here

Learning Objectives

- Objective 1
- Objective 2

Newton's equation of motion

While the electronic structure of atoms is described by quantum mechanics, the motion of atomic nuclei and larger molecules can be described by Newton's laws of motion. Consider two interacting particles as shown in Figure 3.3.A. According to Newton's second law of motion the force acting on a particle is equal to the product of the mass of the particle and its acceleration:

$$\vec{F} = m\vec{a} \tag{3.3.1}$$

where F is the net force acting on a particle with mass m. Equation 3.3.1 describes how a force acting on a body can produce motion of a body. Force and acceleration are both vector quantities. The acceleration is the first derivative of the velocity with respect to time:

$$\vec{a} = \frac{d\vec{v}}{dt} \tag{3.3.2}$$

and the second derivative of the position with respect to time:

$$\vec{a} = \frac{d^2\vec{x}}{dt^2} \tag{3.3.3}$$

As shown in Figure 3.3.A, if two particles interact, they exert forces on one another that are equal in magnitude and opposite in direction, according to Newton's third law.

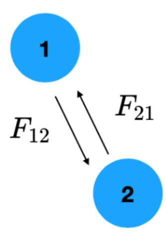

Figure III.3.A. Schematic depiction of two interacting particles. F_{12} is the force acting on particle 2 due to the interaction with particle 1. F_{21} is the equal in magnitude and opposite in direction force on particle 1 due to particle 2.

Given the initial positions and velocities of a system of particles and a suitable expression for the forces acting on each particle, the goal of classical mechanics is to calculate the positions and velocities of the particles at all future times.

Assuming that the potential energy is a function of the atomic positions, $U(\mathbf{R}) = U(R_1, R_2, \ldots, R_N)$, the force is:

$$F(\mathbf{R}) = -\nabla U(\mathbf{R}) \tag{3.3.4}$$

where ∇ is the differential operator:

$$\nabla = \hat{x}\frac{\partial}{\partial x} + \hat{y}\frac{\partial}{\partial y} + \hat{z}\frac{\partial}{\partial z} \tag{3.3.5}$$

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Using Equation 3.3.4 and Equation 3.3.3, Newton's second law can be rewritten as a second order differential equation in terms of the position:

$$-\frac{\partial U(\mathbf{R})}{\partial R_i} = m_i \frac{d^2 \vec{R}_i}{dt^2} \tag{3.3.6}$$

Harmonic motion

As an illustrative example of Newtonian mechanics, consider a body of mass m, attached to a spring, and able to move along the x-direction only as shown in Figure 3.3.B. The potential energy is that of a harmonic oscillator:

$$U(x) = \frac{1}{2} k (x - x_0)^2 \tag{3.3.7}$$

where k is the spring constant that parameterizes the stiffness of the spring. The equilibrium position is when the spring is relaxed and the position of the mass is at x_0. This position corresponds to the minimum in potential energy. The net force acting on the mass at x_0 is zero, meaning that the acceleration is zero at this point, consistent Newton's equation of motion. If the spring is compressed or stretched along the x-axis, the mass will feel a restoring force given by Hook's law:

$$\begin{aligned} F &= -\frac{dU}{dt} \\ F &= -k(x - x_0) \end{aligned} \tag{3.3.8}$$

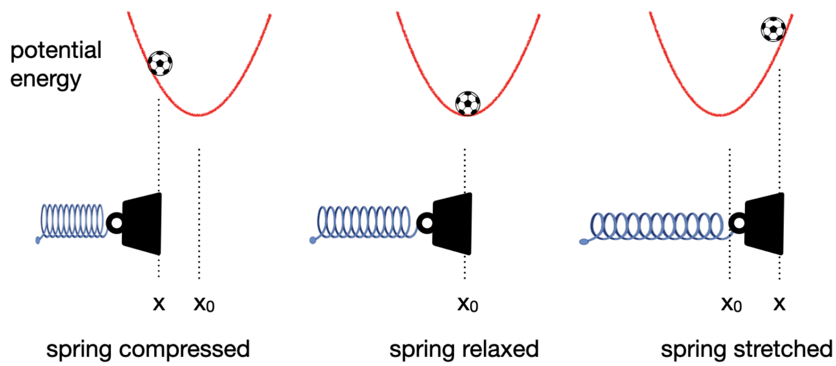

Figure III.3.B. A mass on a spring along the x-direction. The equilibrium position is represented by the position of the mass at x_0 where the spring is relaxed. If the spring is compressed or stretched the mass will feel a restoring force towards the equilibrium position. The potential energy curve is a harmonic oscillator, sketched above showing a minimum at the equilibrium position.

Newton's second law for the harmonic oscillator is:

$$-k(x - x_0) = m \frac{d^2 x}{dt^2} \tag{3.3.9}$$

Equation 3.3.9 is a second order differential equation. The solution for the position as a function of time is

$$x(t) = A \cos(\omega_0 t + \phi) \tag{3.3.10}$$

where A is the amplitude of the oscillation, $\omega_0 = \sqrt{k/m}$, and ϕ is a phase factor that depends on the initial conditions.

Phase space

Equation 3.3.9 is a second order differential equation because the largest derivative order is a second derivative. In general, any n-th order differential equation can be expressed as a n first order differential equations:

$$\begin{aligned} \frac{dx_1}{dt} &= f_1(x_1, \ldots, x_n) \\ &\vdots \\ \frac{dx_n}{dt} &= f_n(x_1, \ldots, x_n) \end{aligned}$$

For the harmonic oscillator, the second order differential Equation 3.3.9 can be equivalently written as two first order differential equations:

$$\frac{dx}{dt} = v(t)$$

$$\frac{dv}{dt} = -\frac{k}{m}(x - x_0) \tag{3.3.11}$$

where $v(t)$ is the velocity. We can completely describe the dynamical state of the system with 2 variables: the position x(t) and the velocity v(t).

Figure 3.3.C shows a plot of Equation 3.3.10 (left) and the phase space plot (right) representing the time evolution of the dynamical system.
