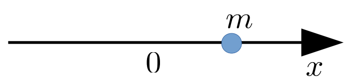
SUMMARY THIRD LECTURE

CONTENTS

I. HAMILTONIAN DYNAMICS

- Hamiltonian dynamics of one particle of mass m (units: kg) on x-axis.



- Definition of position (units: m)

$$x(t) \tag{1}$$

- Definition of velocity (units: $\mathrm{m\,s^{-1}}$)

$$v(t) = \frac{d}{dt}x(t) = \dot{x}(t)\,. \tag{2}$$

- Definition of acceleration (units: $\mathrm{m\,s^{-2}}$)

$$a(t) = \frac{d}{dt}v(t) = \frac{d^2}{dt^2}x(t) = \ddot{x}(t)\,. \tag{3}$$

- Definition of momentum (units: $\mathrm{kg\,m\,s^{-1}}$)

$$p(t) = mv(t) = m\frac{d}{dt}x(t) = m\dot{x}(t)\,. \tag{4}$$

- Definition of force (units: $\mathrm{N = kg\,m\,s^{-2}}$)

$$F(t) = ma(t) = m\frac{d^2}{dt^2}x(t) = m\ddot{r} = \frac{d}{dt}p(t) = \dot{p}(t)\,. \tag{5}$$

- Force and potential energy function (units: J)

$$F = -\frac{d}{dx}V(x)\,. \tag{6}$$

- Kinetic energy (units: J)

$$E_k = \frac{1}{2}mv^2 = \frac{p^2}{2m}\,. \tag{7}$$

- Hamiltonian function or total energy (units: J)

$$\begin{aligned}\mathcal{H}(x,p) &= E_k + V(x) \\ &= \frac{p^2}{2m} + V(x)\,,\end{aligned} \tag{8}$$

- Equations of motion

$$\begin{cases} \dot{x} &= \dfrac{\partial \mathcal{H}}{\partial p} = \dfrac{p(t)}{m} \\ \dot{p} &= -\dfrac{\partial \mathcal{H}}{\partial x} = F(t) = -\dfrac{d}{dx} V(x(t)) \end{cases} . \tag{9}$$

II. HARMONIC OSCILLATOR

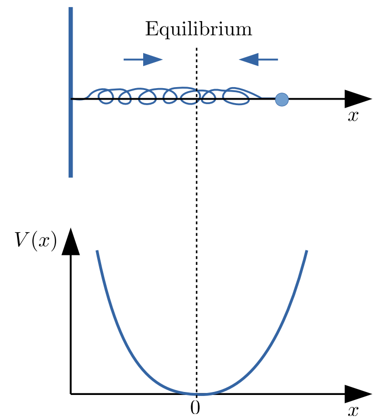
- Potential energy function of an harmonic oscillator:

$$V(x) = \frac{1}{2} k x^2 \, , \tag{10}$$

where k is the spring constant (units: $\mathrm{N\,m^{-1} = kg\,s^{-2}}$).

- Force acting on the mass

$$F = -kx \, . \tag{11}$$



The second equation of the motion of the harmonic oscillator can be written as

$$m\ddot{x} = -kx \, . \tag{12}$$

This is a second-order linear homogeneous ordinary differential equation with constant coefficients and the analytical (exact) solution is

$$x(t) = x(0)\cos(\omega t) + \frac{p(0)}{m\omega}\sin(\omega t) \, , \tag{13}$$

where we introduced the angular frequency of the oscillation (units: $\mathrm{s^{-1}}$)

$$\omega = \sqrt{\frac{k}{m}} \, . \tag{14}$$

Finally, from the first equation of motion

$$p = m\dot{x} \tag{15}$$

we obtain the solution for the momentum

$$p(t) = -m\omega x(0)\sin(\omega t) + p(0)\cos(\omega t) \, . \tag{16}$$

III. EULER INTEGRATOR

The Euler integrator allows to find numerical solutions of the equations of motion. Consider a time interval $[0, \tau]$, and a time-discretization into N_τ sub-intervals $[t_k, t_{k+1}]$ of equal length Δt such that

$$\begin{aligned} t_0 &= 0 \\ t_1 &= \Delta t \\ t_2 &= 2\Delta t \\ &\dots \\ t_{N_\tau} &= \tau = N_\tau \Delta t \end{aligned} \tag{17}$$

The positions and the momenta are updated as

$$
\begin{aligned}
F(t_k) &= -\nabla_r V(x(t_k)) \\
x(t_{k+1}) &= x(t_k) + \frac{p(t_k)}{m}\Delta t + \frac{F(t_k)}{m}\Delta t^2 \\
p(t_{k+1}) &= p(t_k) + F(t_k)\Delta t\,.
\end{aligned}
\tag{18}
$$

where Δt is the integrator timestep.