Essential Notes on Hamiltonian Dynamics

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I. INTRODUCTION

Hamiltonian dynamics is a mathematical framework for describing the behavior of deterministic closed systems over time. It is based on the concept of a mathematical function, the Hamiltonian function, that describes the total energy of a system and is used to derive equations of motion. Hamiltonian dynamics is used in a wide variety of fields, including physics, chemistry, and engineering, to model and analyze the behavior of complex systems.

II. FUNDAMENTAL CONCEPTS

A. Particles in Euclidean space

The object of the study of Hamiltonian dynamics, are dynamical systems, that is, collections of particles with finite mass $m_1, m_2, ..., m_N$ (units: kg). Particles are assumed to be point-like objects in the (three-dimensional) Euclidean space, and their position is denoted by a three-dimensional vector

$$\mathbf{r}_i = \begin{pmatrix} x_i \\ y_i \\ z_i \end{pmatrix} \quad \forall i = 1, 2, ..., N \,, \tag{1}$$

where x, y, z represent the Cartesian coordinates (units: m).

The distance of a particle from the origin $O = (0, 0, 0)$ of the coordinate system is the Euclidean norm

$$\|\mathbf{r}_i\| = \sqrt{x_i^2 + y_i^2 + z_i^2} \,. \tag{2}$$

The distance between two points i and j is

$$d(\mathbf{r}_i, \mathbf{r}_j) = \|\mathbf{r}_i - \mathbf{r}_j\| = \sqrt{(x_i - x_j)^2 + (y_i - y_j)^2 + (z_i - z_j)^2} \,. \tag{3}$$

B. Velocity and acceleration

We now introduce the concept of time, and denote the position of a particle i at time t as $\mathbf{r}(t)$. The average velocity (units: $\mathrm{m\,s^{-1}}$) of a particle between two time steps t_1 and t_2, with $t_2 > t_1$, is given by

$$\bar{\mathbf{v}} = \frac{\mathbf{r}_i(t_2) - \mathbf{r}_i(t_1)}{t_2 - t_1} \tag{4}$$

By taking the limit $t_2 - t_1 \to 0^+$ yields the definition of instantaneous velocity:

$$\mathbf{v}(t) = \lim_{t_2 - t_1 \to 0^+} \frac{\mathbf{r}_i(t_2) - \mathbf{r}_i(t_1)}{t_2 - t_1} = \frac{d}{dt}\mathbf{r}(t) = \dot{\mathbf{r}}(t) \,. \tag{5}$$

The notation $\dot{\mathbf{r}}(t)$ denotes the time derivative of the position.

Likewise, we can define the average and instantaneous acceleration (units: $\mathrm{m\,s^{-2}}$):

$$\mathbf{a}(t) = \lim_{t_2 - t_1 \to 0^+} \frac{\mathbf{v}_i(t_2) - \mathbf{v}_i(t_1)}{t_2 - t_1} = \dot{\mathbf{v}}(t) = \frac{d}{dt}\mathbf{v}(t) = \ddot{\mathbf{r}}(t) \,. \tag{6}$$

The notation $\ddot{\mathbf{r}}(t)$ denotes the second time derivative of the position. Note that both $\mathbf{v}$ and $\mathbf{a}$ are respectively three-dimensional vectors

$$\mathbf{v}_i = \begin{pmatrix} v_{x,i} \\ v_{y,i} \\ v_{z,i} \end{pmatrix} \quad \forall i = 1, 2, ..., N \,, \tag{7}$$

and

$$\mathbf{a}_i = \begin{pmatrix} a_{x,i} \\ a_{y,i} \\ a_{z,i} \end{pmatrix} \quad \forall i = 1, 2, ..., N \,. \tag{8}$$

III. NEWTON'S LAWS OF MOTION

Newton's laws of motion are a set of three fundamental principles that describe the behavior of objects in motion:

1. The law of inertia: A particle at rest tends to stay at rest, and a particle in motion tends to stay in motion with the same speed and in the same direction unless acted upon by an external force.

2. The law of acceleration: The force $\mathbf{F}_i$ (units: N) applied to a particle with mass m_i is directly proportional to the acceleration $\mathbf{a}_i$ of the particle:

$$\begin{aligned} \mathbf{F}_i &= m_i \mathbf{a}_i \\ &= m_i \frac{d}{dt} \mathbf{v}_i \,. \end{aligned} \tag{9}$$

   Note that $\mathbf{F}_i$ is also a three-dimensional vector

$$\mathbf{F}_i = \begin{pmatrix} F_{x,i} \\ F_{y,i} \\ F_{z,i} \end{pmatrix} \quad \forall i = 1, 2, ..., N \,. \tag{10}$$

3. The law of action and reaction: For every action, there is an equal and opposite reaction. This means that when one particle i exerts a force $\mathbf{F}_{ij}$ on another particle j, the second particle j exerts an equal and opposite force $\mathbf{F}_{ji}$ back on the first particle i:

$$\mathbf{F}_{ij} = -\mathbf{F}_{ji} \,. \tag{11}$$

A. Momentum

Newton's laws of motion fully describe the dynamics of the system in terms of positions $\mathbf{r}$ and velocities $\mathbf{v}$. However, it is usually preferable to replace the particle velocity with the particle's momentum (units: $\mathrm{kg\,m\,s^{-1}}$), defined as the product of the velocity and the mass of the particle:

$$\mathbf{p}_i = m_i \mathbf{v}_i \,, \tag{12}$$

with entries

$$\mathbf{p}_i = \begin{pmatrix} p_{x,i} \\ p_{y,i} \\ p_{z,i} \end{pmatrix} \quad \forall i = 1, 2, ..., N \,. \tag{13}$$

Inserting eq. 12 into eq. 9 yields an alternative formula for the second Newton's principle:

$$\mathbf{F}_i = \frac{d}{dt} \mathbf{p}_i \,. \tag{14}$$

Similarly, the third principle (eq. 11) is rewritten as

$$\begin{aligned} \mathbf{F}_{ij} &= -\mathbf{F}_{ji} \\ \frac{d}{dt} \mathbf{p}_j &= -\frac{d}{dt} \mathbf{p}_i \,, \end{aligned} \tag{15}$$

where $\mathbf{p}_j$ is the momentum of the particle j due to the force $\mathbf{F}_{ij}$ exerted by the particle i, and $\mathbf{p}_i$ is the momentum of the particle i due to the force $\mathbf{F}_{ji}$ exerted by the particle j. It follows that

$$\frac{d}{dt} (\mathbf{p}_j + \mathbf{p}_i) = 0 \,, \tag{16}$$

and

$$\mathbf{p}_j + \mathbf{p}_i = \text{const.} \,. \tag{17}$$

Eq. 17 is known as the law of conservation of momentum and can be generalized to $N > 2$ particles interacting in a closed system (i.e. a system that does not exchange matter and energy with the external environment):

$$\sum_{i=1}^{N} \mathbf{p}_i = \text{const.}. \tag{18}$$

Considering this important principle, it makes sense to change velocity to momentum as the fundamental coordinate of motion in order to simplify the analysis of systems involving multiple interacting objects. For example, in collisions, we can use the conservation of momentum to calculate the velocities of the objects after the collision, without needing to know the details of the collision process itself.

B. Force and potential energy

Consider now a particle that can move only along the x-direction, and assume that this particle is connected to a spring. The force acting on the particle, along the x-direction, is given by Hook's law

$$F_x(x) = -kx\,, \tag{19}$$

where the spring constant k depends on the physical characteristics of the spring. Eq. 19 can also be written as a derivative of a parabola:

$$\begin{aligned} F_x(x) &= -kx \\ &= -\frac{d}{dx}\left(\frac{1}{2}kx^2\right) \\ &= -\frac{d}{dx}V(x)\,. \end{aligned} \tag{20}$$

This function is referred to as the potential energy function of a one-dimensional spring (or a one-dimensional harmonic oscillator):

$$V(x) = \frac{1}{2}kx^2\,. \tag{21}$$

From a physical point of view, the function $V(x) : \mathbb{R} \to \mathbb{R}$ represents the potential energy (units: J) of the particle at a given position $\mathbf{r}$. When $x = 0$, the derivative of the potential energy of the harmonic oscillator is zero. This is the bottom of the parabola and corresponds to the equilibrium point: no force acts on the particle. If $x < 0$, the spring is compressed, and the mass is in the left region of the parabola, where the derivative is negative. Here, the force assumes a positive value and pushes the mass toward the right side of the parabola. Vice versa, if $x > 0$, the parabola derivative is positive, and the force, negative, pushes the mass on the left side of the parabola.

If we consider a particle moving in the three-dimensional space, the force acting on it is determined by the three-dimensional potential energy function $V(\mathbf{r}) : \mathbb{R}^3 \to \mathbb{R}$:

$$\mathbf{F}(\mathbf{r}) = -\nabla V(\mathbf{r})\,. \tag{22}$$

Note that $\mathbf{F}(\mathbf{r}) : \mathbb{R}^3 \to \mathbb{R}^3$ is a three-dimensional vector with entries:

$$\begin{cases} F_x(\mathbf{r}) = -\dfrac{\partial}{\partial x}V(\mathbf{r}) \\ F_y(\mathbf{r}) = -\dfrac{\partial}{\partial y}V(\mathbf{r}) \\ F_z(\mathbf{r}) = -\dfrac{\partial}{\partial z}V(\mathbf{r}) \end{cases} . \tag{23}$$

In eq. 22, the object ∇V is called the gradient of the potential and the symbol ∇ is the operator nabla:

$$\nabla = \left(\frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z}\right)\,, \tag{24}$$

which calculates the partial derivatives, i.e. the derivatives in each dimension x, y, and z, of the three-dimensional function $V(\mathbf{r})$. The symbol $\frac{\partial}{\partial x}$ is equivalent to $\frac{d}{dx}$, but preferred when a function depends on more variables.

Alternative notations for eq. 22 are

$$\mathbf{F}(\mathbf{r}) = -\nabla_{\mathbf{r}} V(\mathbf{r}), , \tag{25}$$

and

$$\mathbf{F}(\mathbf{r}) = -\frac{\partial}{\partial \mathbf{r}} V(\mathbf{r}), , \tag{26}$$

If the system is made of N particles, the potential energy function is a $3N$-dimensional function $V(\mathbf{r}_1, \mathbf{r}_2, ..., \mathbf{r}_N) : \mathbb{R}^{3N} \to \mathbb{R}$ and the force acting on each particle is

$$\mathbf{F}_i(\mathbf{r}_1, \mathbf{r}_2, ..., \mathbf{r}_N) \;=\; -\nabla_i V(\mathbf{r}_1, \mathbf{r}_2, ..., \mathbf{r}_N)\,, \tag{27}$$

the symbol $\nabla_i V$ denotes the gradient with respect the coordinates of the particle i.

Here, we will work only with forces that can be written in terms of a potential energy function. These forces are called conservative, for example, the force of a spring, gravity, the Coulomb force, and the van der Waals force. However, there exist also non-conservative forces that cannot be defined by a potential function.

C. Kinetic energy

Kinetic energy (units: J) is a form of energy that an object possesses because it is moving. If we consider a particle moving on the x-axis, then the formula for kinetic energy is:

$$E_k = \frac{1}{2} m v_x^2 = \frac{p_x^2}{2m}\,. \tag{28}$$

Then the greater the mass and velocity of an object, the greater its kinetic energy. If the particle can move in the three-dimensional space, the kinetic energy is

$$E_k = \frac{1}{2} m \mathbf{v}^2 = \frac{\mathbf{p}^2}{2m}\,. \tag{29}$$

Note that $\mathbf{v}^2$ and $\mathbf{p}^2$ in eq. 32 are squares of vectors, and have to be calculated as dot-products:

$$\mathbf{v}^2 = \mathbf{v} \cdot \mathbf{v} = v_x^2 + v_y^2 + v_z^2\,, \tag{30}$$

and

$$\mathbf{p}^2 = \mathbf{p} \cdot \mathbf{p} = p_x^2 + p_y^2 + p_z^2\,, \tag{31}$$

If the system is made of N particles, the kinetic energy of the full system is the sum of the kinetic energy of each particle:

$$\begin{aligned} E_k \;&=\; \sum_{i=1}^{N} \frac{1}{2} m_i \mathbf{v}_i^2 = \frac{1}{2} m_1 \mathbf{v}_1^2 + \frac{1}{2} m_2 \mathbf{v}_2^2 + ... + \frac{1}{2} m_N \mathbf{v}_N^2 \\ &=\; \sum_{i=1}^{N} \frac{\mathbf{p}_i^2}{2m_i} = \frac{\mathbf{p}_1^2}{2m_1} + \frac{\mathbf{p}_2^2}{2m_2} + ... + \frac{\mathbf{p}_N^2}{2m_N}\,. \end{aligned} \tag{32}$$

D. Hamiltonian function and equations of motion

The Hamiltonian function describes the total energy of the system, it is given by the sum of kinetic energy and potential energy:

$$\mathcal{H} = E_k + V\,. \tag{33}$$

The value of the Hamiltonian function depends on the position and momentum of the particles, which can change over time. If the potential energy function depends only on the position of the particles, then the Hamiltonian function, i.e.

the total energy of the system, is constant along the trajectory of the system. The Hamiltonian function is important in classical mechanics because it can be used to derive the equations of motion of the system, which describe how the positions and velocities of the particles in the system change over time.

Consider now a single particle moving along the x-axis, then the Hamiltonian function is

$$\mathcal{H}(x, p_x) = \frac{p_x^2}{2m} + V(x)\,, \tag{34}$$

and the equation of motion are

$$\begin{cases} \dot{x} &= \frac{\partial \mathcal{H}}{\partial p_x} = \frac{p_x(t)}{m} \\ \dot{p_x} &= -\frac{\partial \mathcal{H}}{\partial x} = F_x(t) = -\nabla V(x(t)) \end{cases} . \tag{35}$$

The Hamiltonian function of a system with a single particle moving in Euclidean space is

$$\mathcal{H}(\mathbf{r}, \mathbf{p}) = \frac{\mathbf{p}^2}{2m} + V(\mathbf{r})\,, \tag{36}$$

and the equation of motion are

$$\begin{cases} \dot{\mathbf{r}} &= \frac{\partial \mathcal{H}}{\partial \mathbf{p}} = \frac{\mathbf{p}(t)}{m} \\ \dot{\mathbf{p}} &= -\frac{\partial \mathcal{H}}{\partial \mathbf{r}} = -\nabla V(\mathbf{r}(t)) = \mathbf{F}(t) \end{cases} . \tag{37}$$

Note that the notation $\frac{\partial \mathcal{H}}{\partial \mathbf{p}}$ denotes the derivatives with respect to p_x, p_y and p_z, while the notation and $\frac{\partial \mathcal{H}}{\partial \mathbf{r}}$ denotes the derivatives with respect to x, y and z.

The Hamiltonian function of a system with N particles moving in Euclidean space is

$$\mathcal{H}(\mathbf{r}_1, \mathbf{r}_2, ..., \mathbf{r}_N, \mathbf{p}_1, \mathbf{p}_2, ..., \mathbf{p}_N) = \sum_{i=1}^{N} \frac{\mathbf{p}_i^2}{2m_i} + V(\mathbf{r}_1, \mathbf{r}_2, ..., \mathbf{r}_N)\,, \tag{38}$$

and the equation of motion for a particle i are

$$\begin{cases} \dot{\mathbf{r}}_i &= \frac{\partial \mathcal{H}}{\partial \mathbf{p}_i} = \frac{\mathbf{p}_i(t)}{m_i} \\ \dot{\mathbf{p}}_i &= -\frac{\partial \mathcal{H}}{\partial \mathbf{r}_i} = -\nabla_i V(\mathbf{r}_1(t), \mathbf{r}_2(t), ..., \mathbf{r}_N(t)) = \mathbf{F}_i(t) \end{cases} . \tag{39}$$

IV. HARMONIC OSCILLATOR

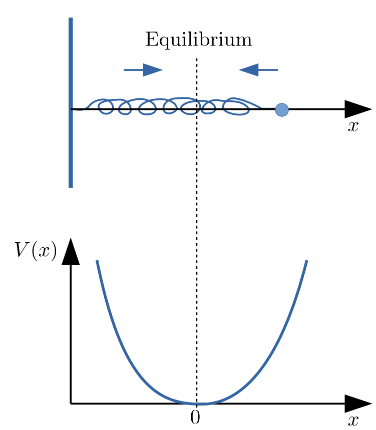
- Potential energy function of an harmonic oscillator:

$$V(x) = \frac{1}{2}kx^2\,, \tag{40}$$

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

- Force acting on the mass

$$F = -kx\,. \tag{41}$$



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

$$m\ddot{x} = -kx\,. \tag{42}$$

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

$$x(t) = x(0)\cos(\omega t) + \frac{p(0)}{m\omega}\sin(\omega t)\,, \tag{43}$$

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

$$\omega = \sqrt{\frac{k}{m}}\,. \tag{44}$$

Finally, from the first equation of motion

$$p = m\dot{x} \tag{45}$$

we obtain the solution for the momentum

$$p(t) = -m\omega x(0)\sin(\omega t) + p(0)\cos(\omega t)\,. \tag{46}$$