Mechanics

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Chapter 1

Hamilton's equation of motion

1.1 Introduction

These are the lecture notes of the course "Mechanics, Electricity, and Magnetism 2", as given in the first quarter of 2026, covering the mechanics part. Last year's lecture notes, which are still available, summarized the main equations and ideas of Newtonian mechanics as discussed in the text book (Serway [1]), chapters 9-14.

These lecture notes treat the same topics, but the approach is different. Rather than taking Newton's laws as the starting point and solving problems step by step from there, we use a "top-down" approach. The focus is on simplifying the problem first by using conservation laws for energy, linear momentum, and angular momentum, whenever they apply, and by rewriting the problem using a center-of-mass frame. We achieve this by introducing Hamilton's classical equations of motion and we use them whenever they are simpler than Newton's. In a physics curriculum, this is taught in a course on analytical mechanics. This course, however, targets chemistry students, and it is not a course on analytical mechanics. Rather than taking the long road from Lagrangian, Euler-Lagrange equations, and the principle of least action, we'll take some short cuts to where these strictly speaking advance concepts make life easier. The goal it to prepare for subsequent chemistry courses on quantum mechanics, chemical bonding, and statistical mechanics, where the use of these concepts is essential. In particular, we believe that Hamilton's classical equations of motion will ease the switch to quantum mechanics.

1.2 A brief history

These are some important names and dates:

1687 Isaac Newton, 2nd law, relating force $\boldsymbol{F}$, mass m, and acceleration

$$\boldsymbol{F} = m\boldsymbol{a}. \tag{1.1}$$

1788 Joseph-Louis Lagrange, introducing the Lagrangian

$$L = T - V, \tag{1.2}$$

where T is the kinetic energy (T from "travail mechanique") and V is potential energy.

1830 William Rowan Hamilton, introducing the Hamiltonian

$$H = T + V \tag{1.3}$$

1915 Emmy Noether: Noether's theorem relating continuous symmetries to conservation laws for energy, momentum, and angular momentum.

1925 Erwin Schrödinger, Schrödinger equation

$$i\hbar\frac{d}{dt}\Psi = \hat{H}\Psi \tag{1.4}$$

and its time independent version

$$\hat{H}\Psi = E\Psi. \tag{1.5}$$

1.3 Trajectory of projectile using Newton's laws

From mechanics I you may remember how a particle with mass m under gravity follows a parabolic flight. The position of the particles is given by Cartesian coordinates (x, y), with x the horizontal component and y the vertical component. The trajectory of the particle is described by the time (t) dependent positions, $[x(t), y(t)]$. The time derivative of the position is the velocity,

$$v_y = \dot{y} \equiv \frac{d}{dt}y(t), \tag{1.6}$$

and the time derivative of the velocity is the acceleration

$$a_y = \dot{v}_y \equiv \frac{d}{dt}v_y(t) = \ddot{y}. \tag{1.7}$$

Similarly, for the horizontal component we have velocity v_x and acceleration a_x.

Newton's second law for the vertical component is

$$F_y = ma_y, \tag{1.8}$$

where F_y is the force due to gravity

$$F_y = -mg, \tag{1.9}$$

and so we have $a_y = -g$. Solving the equation of motion gives

$$y(t) = y(0) + v_y(0)t - \frac{1}{2}gt^2. \tag{1.10}$$

For the horizontal component there is no force, so

$$a_x = 0, \tag{1.11}$$

and the velocity $v_x = v_x(0)$ is constant, so we find

$$x(t) = x(0) + v_x t. \tag{1.12}$$

Thus, if the initial position $[x(0), y(0)]$ and the initial velocities $[v_x(0), v_y(0)]$ are given, the full trajectory is known.

1.4 Potential energy and kinetic energy

The force of gravity is **conservative**, which means it can be integrated to define a **potential energy** $V(x, y)$. The forces depend on minus the derivatives in x and y direction

$$F_x = -\frac{\partial}{\partial x}V(x, y) \tag{1.13}$$

$$F_y = -\frac{\partial}{\partial y}V(x, y), \tag{1.14}$$

where we use the notation for partial derivatives, since the potential is a function of all coordinates.

Since the horizontal component of the force is zero, the potential only depends on y,

$$V(x, y) = -gy. \tag{1.15}$$

We have the freedom to add a constant value to the potential, since that does not affect the forces.

The **kinetic energy** depends on the velocity of the particle, $v \equiv \sqrt{v_x^2 + v_y^2}$,

$$T = \frac{1}{2}mv^2 = \frac{1}{2}m(v_x^2 + v_y^2). \tag{1.16}$$

1.5 Linear momentum

Newton defined "quantity of motion", which we now call linear momentum. It's Cartesian components are given by

$$p_x = mv_x \tag{1.17}$$
$$p_y = mv_y. \tag{1.18}$$

Newton's second law can be expressed in terms of linear momenta,

$$\dot{p}_x = F_x, \tag{1.19}$$
$$\dot{p}_y = F_y, \tag{1.20}$$

and this is actually how it was done in his book *Principia Mathematica* (1687).

1.6 Hamiltonian mechanics

The power of Hamiltonian mechanics is that the equations of motion look the same in any coordinate system. First, however, we will apply the method to the (Cartesian) y coordinate of the above problem, in which case it is easy to see that it is equivalent to Newton's approach. However, we will denote the coordinate as $q = y$ to stress the fact that this is the Hamiltonian approach for any system where to position can be described by a single coordinate. In this notation, the velocity is written as $\dot{q} = v_y$.

Step 1: Write down the kinetic energy using velocities,

$$T = \frac{1}{2}m\dot{q}^2. \tag{1.21}$$

Step 2: Define the momentum **conjugate** to the velocity as derivative of the kinetic energy with respect to the velocity

$$p \equiv \frac{\partial}{\partial y}T = m\dot{q}. \tag{1.22}$$

In this case, clearly $p = p_y$. However, the analogous definition of **conjugate** momenta applies in any coordinate system.

Step 3: Rewrite the kinetic energy using the conjugate momenta

$$T = \frac{p^2}{2m}. \tag{1.23}$$

Step 4: Write down the **Hamiltonian**, which is the expression for the total energy using coordinates and their conjugate momenta, so in this case

$$H(q,p) = T(p) + V(q) \tag{1.24}$$
$$= \frac{p^2}{2m} + mgq.$$

Step 5: The equations of motion for position q and conjugate momentum p are

$$\dot{q} = \frac{\partial}{\partial p}H(p,q) \tag{1.25}$$
$$\dot{p} = -\frac{\partial}{\partial q}H(p,q). \tag{1.26}$$

The first of these equations give $\dot{q} = p/m$, which matches the definition of the momentum. Since only the potential depends on the coordinate, the second equation reproduces Newton's second law

$$\dot{p} = -\frac{\partial}{\partial q}V(q) = F_y. \tag{1.27}$$

In the next section we consider an example where the difference between Newton and Hamilton becomes a little clearer.

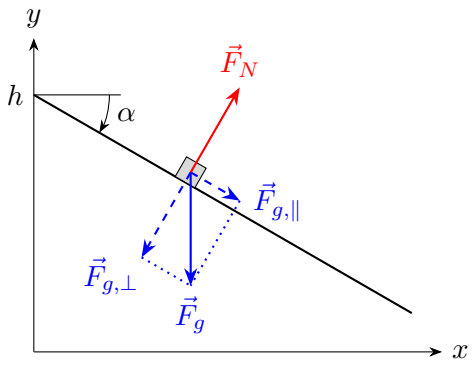

Figure 1.1: Particle on a slope.

1.7 Degrees of freedom and constraints

The problem of a parabolic trajectory given above is a problem with two **degrees of freedom**, i.e., the coordinates x and y. These Cartesian coordinates are particularly convenient in this case, because it splits the problem into two problems with one degree of freedom, i.e., horizontal motion and vertical motion.

For a particle sliding down a slope with a given angle relative to the horizontal (α), its position is still given by Cartesian coordinates (x, y) but it has only one degree of freedom, because if coordinate x is known and it is known that the particle is on the slope, than one can compute its y coordinate and *vice versa*, so there is really only one "free" coordinate. In Newtonian mechanics, this problem is solved by writing the force of gravity as the sum of a force parallel to the surface, $F_\parallel$ and a force perpendicular to the surfaces, $F_\perp$, and adding a **reactive force** which counteracts the perpendicular component of gravity, see Fig. 1.1. Thus, the total force on the particles is $\vec{F}_{g,\parallel}$. This vector has an x and a y component,

$$F_{g,\parallel,x} = \cos(\alpha)F_{g,\parallel} = -\cos(\alpha)\sin(\alpha)mg \quad (1.28)$$
$$F_{g,\parallel,z} = \sin(\alpha)F_{g,\parallel} = -\sin(\alpha)\sin(\alpha)mg \quad (1.29)$$

where we take α to be a negative angle for the slope shown in the figure. It is left as an exercise to solve Newton's second law for both components and to show that if initially the particle was at rest at $(0, h)$ its trajectory is given by

$$x(t) = \frac{1}{2}g\cos(\alpha)\sin(\alpha)t^2 \quad (1.30)$$
$$y(t) = h + \frac{1}{2}g\sin(\alpha)\sin(\alpha)t^2. \quad (1.31)$$

As a quick check note that the velocities are

$$v_x(t) = g\cos(\alpha)\sin(\alpha)t \quad (1.32)$$
$$v_y(t) = g\sin(\alpha)\sin(\alpha)t, \quad (1.33)$$

so for $\alpha = 0$ the velocities are zero, and otherwise $v_y/v_x = \tan\alpha$.

If $\alpha = 0$ the slope is horizontal and we have $\sin\alpha = 0$. We will now present an alternative method to solve this problem.

1.8 Particle on a slope

In Hamiltonian mechanics we do not start with considering the forces. Instead, for this one-degree-of-freedom problem, we define a single coordinate $r(t)$ that gives the position of the particle,

$$x(t) = r(t)\cos\alpha \quad (1.34)$$
$$y(t) = h + r(t)\sin\alpha. \quad (1.35)$$

The time dependence was explicitly included, to make clear that the initial height h and angle of the slope α are constants which we assume to be given. Thus, the trajectory is given by $r(t)$. We now follow again the give steps given above

1: Kinetic energy as function of velocity

From the above definition we have

$$v_x(t) = \dot{r}\cos\alpha \tag{1.36}$$
$$v_y(t) = \dot{r}\sin\alpha, \tag{1.37}$$

so the kinetic energy as function of $\dot{r}$ is

$$\begin{aligned} T &= \frac{1}{2}m(v_x^2 + v_y^2) \\ &= \frac{1}{2}m(\dot{r}^2\cos^2\alpha + \dot{r}^2\sin^2\alpha) \\ &= \frac{1}{2}m\dot{r}^2. \end{aligned} \tag{1.38}$$

2: Define conjugate momenta

The momentum conjugate to r is

$$p_r = \frac{\partial}{\partial\dot{q}}T(\dot{r}) = m\dot{r}, \tag{1.39}$$

which is still something you would have gotten with Newton's definition of momentum.

3: Kinetic energy using momenta

Using the conjugate momentum we have

$$T(p_r) = \frac{p_r^2}{2m}. \tag{1.40}$$

4: Write down the Hamiltonian

In Cartesian coordinates, the potential was $V(z) = mgy$, so now we have

$$V(r) = mg(h + r\sin\alpha) \tag{1.41}$$

and the Hamiltonian for this problem is

$$H(r, p_r) = \frac{p_r^2}{2m} + mg(h + r\sin\alpha). \tag{1.42}$$

5: Hamilton's equation of motion

For coordinate $r(t)$ and momentum $p_r(t)$, we have

$$\dot{r} = \frac{\partial}{\partial p_r}H(r, p_r) = \frac{p_r}{m} \tag{1.43}$$
$$\dot{p}_r = -\frac{\partial}{\partial r}H(r, p_r) = -mg\sin\alpha. \tag{1.44}$$

Taking the time derivative of the first equation, using the second gives

$$\ddot{r} = \frac{\dot{p}_r}{m} = g\sin\alpha. \tag{1.45}$$

If, as before, we assume that the particle is initially at rest at $(0, h)$, which corresponds to $r(0) = 0$ and $\dot{r}(0) = 0$ we find

$$r(t) = \frac{1}{2}g\sin(\alpha)\, t^2. \tag{1.46}$$

Putting this back into Eqs. (1.34) and (1.35) gives the same trajectory we found with Newton [Eqs. (1.30) and (1.31)].

1.9 Generalized coordinates

The carbon monoxide molecule, CO, the most abundant heteronuclear molecule in the universe, consists of two atoms. The positions of its atoms can be described using Cartesian coordinates, (x_i, y_i, z_i), with, e.g., $i = \mathrm{C}$ for the carbon atom, and $i = \mathrm{O}$ for the oxygen atom, so this molecule has six degrees of freedom if we treat the atoms as point particles. Depending on the problem, other coordinates may be more convenient. For example to study the motion of the molecule under gravitational forces, we could use the center-

of-mass coordinates, (X, Y, Z),

$$X \equiv \frac{m_{\rm C} x_{\rm C} + m_{\rm O} x_{\rm O}}{m_{\rm C} + m_{\rm O}}, \tag{1.47}$$

$$Y \equiv \frac{m_{\rm C} y_{\rm C} + m_{\rm O} y_{\rm O}}{m_{\rm C} + m_{\rm O}}, \tag{1.48}$$

$$Z \equiv \frac{m_{\rm C} z_{\rm C} + m_{\rm O} z_{\rm O}}{m_{\rm C} + m_{\rm O}}. \tag{1.49}$$

To describe the interatomic potential and vibrational motion we would use the distance r between the atoms, and to described rotation of the molecule we could use the spherical polar angles (θ, ϕ).

The six coordinates $(X, Y, Z, r, \theta, \phi)$ are an example of **generalized coordinates**. Hamilton's equations of motion are particularly useful for working with generalized coordinates, since the have the same form in any coordinate system.

To describe a particle sliding down a slope, we actually already used a special case of these generalized coordinates, and they have other important applications. For example, they can be used to describe the orbits of planets, the collisions of two particles, or, e.g. the motion of in electron in the Bohr model for the hydrogen atom.

Since these coordinates have several applications, we here give their explicit relation to Cartesian coordinates. For compactness, we switch to vector notation. For the Cartesian coordinates of the atoms we use two vectors,

$$\boldsymbol{r}_i = \begin{pmatrix} x_i \\ y_i \\ z_i \end{pmatrix}, \quad i = {\rm C}, {\rm O}, \tag{1.50}$$

so the c.o.m. can be written as

$$\boldsymbol{X} = \frac{m_C \boldsymbol{r}_C + m_O \boldsymbol{r}_O}{m_C + m_O}. \tag{1.51}$$

The coordinates (r, θ, ϕ) are related to the vector $\boldsymbol{r}$, which points from C to O,

$$\boldsymbol{r} \equiv \boldsymbol{r}_O - \boldsymbol{r}_C = \begin{pmatrix} x \\ y \\ z \end{pmatrix} = r \begin{pmatrix} \cos\phi \sin\theta \\ \sin\phi \sin\theta \\ \cos\theta \end{pmatrix}, \tag{1.52}$$

so that $r = |\boldsymbol{r}| = \sqrt{x^2 + y^2 + z^2}$ is the length of the vector $\boldsymbol{r}$.

If the generalized coordinates are given, i.e., we know $\boldsymbol{X}$ and $\boldsymbol{r}$, the Cartesian coordinates of the atoms are

$$\boldsymbol{r}_{\rm C} = \boldsymbol{X} - \frac{m_{\rm O}}{m_{\rm C} + m_{\rm O}} \boldsymbol{r} \tag{1.53}$$

$$\boldsymbol{r}_{\rm O} = \boldsymbol{X} + \frac{m_{\rm C}}{m_{\rm C} + m_{\rm O}} \boldsymbol{r}. \tag{1.54}$$

To verify these equations substitute them into Eqs. (1.51) and into Eq. (1.52).

Another example of generalized coordinates are bond lengths, bond angles, and torsion angles to describe the geometry of molecules.

1.10 Hamilton's equations of motion in more dimensions

If we have N generalized coordinates $\{q_i, i = 1, 2, \ldots, N\}$, and a kinetic energy depending on these coordinates ($\boldsymbol{q}$ in vector notation) and their time derivatives $\dot{\boldsymbol{q}}$, i.e. the velocities, then the conjugate momenta are defined by

$$p_i \equiv \frac{\partial T(\boldsymbol{q}, \dot{\boldsymbol{q}})}{\partial \dot{q}_i}. \tag{1.55}$$

With the Hamiltonian expressed as a function of the coordinates $\boldsymbol{q}$ and the vector of conjugate

momenta the Hamilton's equation of motion are

$$\dot{q}_i = \frac{\partial H(\boldsymbol{q}, \boldsymbol{p})}{\partial p_i} \tag{1.56}$$

$$\dot{p}_i = -\frac{\partial H(\boldsymbol{q}, \boldsymbol{p})}{\partial q_i}. \tag{1.57}$$

In the example of the parabolic flight in the (x, y) plane, we have $N = 2$, $\boldsymbol{q} = (q_1, q_2) = (x, y)$ and the Hamiltonian

$$H(\boldsymbol{q}, \boldsymbol{p}) = \frac{p_1^2}{2m} + \frac{p_2^2}{2m} + V(q_2). \tag{1.58}$$

In this example the potential only depends on $q_2 = y$, and the Hamiltonian can be written as the sum of two Hamiltonians that depend on different coordinates,

$$H(\boldsymbol{q}, \boldsymbol{p}) = H(q_1, p_1) + H(q_2, p_2). \tag{1.59}$$

By writing down the equations of motion, we see that, as with Newton, the problem splits in two independent parts, one for coordinate 1 (x) and one for coordinate 2 (y). This is important to remember: when we can write the Hamiltonian as a sum of terms depending on different coordinates, the problem simplifies tremendously.

Chapter 2

Collision of two particles

2.1 Motion in 1D

For two particles with masses m_1 and m_2, moving on a straight line with positions x_1 and x_2, the Hamiltonian is

$$H = \frac{p_1^2}{2m_1} + \frac{p_2^2}{2m_2} + V(x_2 - x_1), \tag{2.1}$$

where we introduce a potential V. We may think of the particles as tennis balls, and the coordinates x_1 and x_2 the centers of these balls. In that case, if the "particles" are further apart then the sum of the radii of the balls, the potential is zero, and if they get closer, the potential will go up. We assume that the potential depends on the distance between the particles

$$r \equiv x_2 - x_1, \tag{2.2}$$

so we may write

$$V(x_2 - x_1) = V(r). \tag{2.3}$$

If initially $x_2 > x_1$ then r is positive, and the potential could look like shown in Fig. (2.1).

From Hamilton's equation of motion we have

$$\dot{p}_1 = -\frac{\partial}{\partial x_1} V(r) = -\frac{\partial r}{\partial x_1} V'(r) = V'(r), \tag{2.4}$$

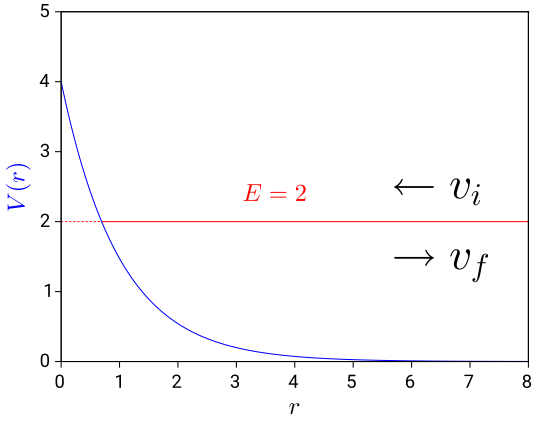

Figure 2.1: Potential for colliding particles (blue curve). The motion before the collision is indicated by $v_i < 0$. After the collision it is $v_f > 0$. The total internal energy is $E = 2$ (arbitrary units).

where

$$V'(r) = \frac{d}{dr}V(r). \tag{2.5}$$

For the other particle we have

$$\dot{p}_2 = -\frac{\partial}{\partial x_2}V(r) = -\frac{\partial r}{\partial x_2}V'(r) = -V'(r) \tag{2.6}$$

so

$$\dot{p}_1 + \dot{p}_2 = 0. \tag{2.7}$$

Thus, the total linear momentum

$$P = p_1 + p_2 = m_1 v_1 + m_2 v_2, \tag{2.8}$$

is conserved. This is an example of Noether's theorem, which relates continuous symmetries, in this case translational symmetry, to a conserved quantity, in this case linear momentum. Translational symmetry means that the "physics", i.e., the equations of motion, do not change under the transformation $x_1 \to x_1 + \Delta$, $x_2 \to x_2 + \Delta$, where Δ is the shift. In Hamiltonian mechanics, the equations of motion are fully determined by the Hamiltonian, so we just have to check that the Hamiltonian is indeed invariant under this transformation. Since only the potential depends on the coordinates, we just have to verify that it is invariant, i.e.,

$$V[(x_1 + \Delta) - (x_1 + \Delta)] = V(x_2 - x_2) = V(r). \tag{2.9}$$

We now solve this collision problem using the generalized coordinates (X, r), with X the c.o.m.,

$$X \equiv \frac{m_1 q_1 + m_2 q_2}{m_1 + m_2}. \tag{2.10}$$

As for the CO molecule [Eqs. (1.53) and (1.54)], we can express the Cartesian coordinates in the generalized coordinates

$$x_1 = X - \frac{m_2}{m_1 + m_2}r \tag{2.11}$$

$$x_2 = X + \frac{m_1}{m_1 + m_2}r. \tag{2.12}$$

To find the conjugate momenta, we start by writing the kinetic energy in velocities,

$$\begin{aligned} T =& \frac{1}{2}m_1\dot{x}_1^2 + \frac{1}{2}m_2\dot{x}_2^2 \\ =& \frac{1}{2}m_1(\dot{X} - \frac{m_2}{m_1 + m_2}\dot{r})^2 \\ &+ \frac{1}{2}m_2(\dot{X} + \frac{m_1}{m_1 + m_2}\dot{r})^2. \end{aligned} \tag{2.13}$$

After some algebra, we find

$$T = \frac{1}{2}M\dot{X}^2 + \frac{1}{2}\mu\dot{r}^2, \tag{2.14}$$

where the total mass M, and the reduced mass μ are given by

$$M = m_1 + m_2 \tag{2.15}$$

$$\mu = \frac{m_1 m_2}{m_1 + m_2}. \tag{2.16}$$

The momentum conjugate to the c.o.m. coordinate is

$$P_X = \frac{\partial}{\partial \dot{X}}T(\dot{X}, \dot{r}) = M\dot{X} \tag{2.17}$$

From the expression of the c.o.m. [Eq. 2.10)] we find

$$\begin{aligned} M\dot{X} &= M\frac{m_1 v_1 + m_2 v_2}{m_1 + m_2} \\ &= m_1 v_1 + m_2 v_2 = P, \end{aligned} \tag{2.18}$$

so the **moment conjugate to the c.o.m. coordinate is the total linear momentum**, $P_X = P$.

For the moment conjugate to r we find

$$p_r = \frac{\partial}{\partial \dot{r}}T(\dot{X}, \dot{r}) = \mu\dot{r}. \tag{2.19}$$

so the Hamiltonian is given by

$$H(X, r, P, p_r) = \frac{P^2}{2M} + \frac{p_r^2}{2\mu} + V(r), \tag{2.20}$$

which can be written as the sum of two Hamiltonians of different coordinates

$$H(X, r, P, p_r) = H_{\text{com}}(X, P) + H_r(r, p_r), \quad (2.21)$$

with

$$H_{\text{com}}(X, P) = \frac{P^2}{2M} \quad (2.22)$$

$$H_{\text{com}}(X, P) = \frac{p_r^2}{2\mu} + V(r). \quad (2.23)$$

Thus, the c.o.m. motion corresponds to the motion of a free particle with mass M, and the relative motion is equivalent to a single particle with mass μ experiencing a potential $V(r)$.

Since the c.o.m. Hamiltonian does not depend on X, linear momentum P, and hence $\dot{X}$ are conserved. Thus we can solve the c.o.m. motion

$$X(t) = X(0) + \dot{X}t, \quad (2.24)$$

where we can compute the velocity if the initial velocities are known,

$$\dot{X} = \frac{P}{M} = \frac{m_1 v_{1,i} + m_2 v_{2,i}}{M}. \quad (2.25)$$

The **internal motion**, $r(t)$ depends on the potential, but sufficiently long before (r_i) and after (r_f) the collision we assume $V(r_i) = V(r_f) = 0$. The initial relative velocity is, from taking the derivative of Eq. (2.2)

$$v_{r,i} = \dot{r}_i = \dot{x}_{2,i} - \dot{x}_{1,i} = v_{2,i} - v_{1,i}, \quad (2.26)$$

and since the internal energy is conserved, but the velocity changes sign, we must have

$$v_{r,f} = -v_{r,i}. \quad (2.27)$$

To find the velocities in the lab frame after the collision, $\dot{x}_{1,f}$ and $\dot{x}_{2,f}$, we take the time derivatives of Eqs. (2.11) and (2.12),

$$v_1 = \dot{X} - \frac{m_2}{M}\dot{r} \quad (2.28)$$

$$v_2 = \dot{X} + \frac{m_1}{M}\dot{r} \quad (2.29)$$

and plug in the values of $\dot{X}$ and $v_{r,f}$.

If the potential $V(r)$ is given, e.g., as in Fig. (2.1), we can check whether it is actually sufficiently repulsive to make the relative velocity change sign. We compute the internal energy $E = \frac{1}{2}\mu v_{r,i}^2$. If for some distance r we have $V(r) > E$ then the relative velocity will change sign, and otherwise not. The value of r where $V(r) = E$ is called the **classical turning point**. Here "classical" refers to "classical mechanics", since in quantum mechanics it can be different due to a phenomenon called "tunneling", where a particle can temporarily be in a **classical forbidden region** where $V(r) > E$.

2.2 Inelastic collisions

Strictly, with Hamilton's equation of motion, we have assumed the forces are conservative, and energy is conserved, so it seems the derivation so far only applies to **elastic collisions**.

If we assume that the forces are **non-conservative** at some short distance $r_{\min}$, the motion for $r < r_{\min}$ cannot be described by a potential $V(r)$. Thus, the above derivation still holds, until time t_f, where $r_f = r_{\min}$. If at that point the relative motion stops, $v_{r,f} = 0$, so also $p_{r,f} = 0$, the **internal energy is lost**, $E(t_f) = 0$. Still, we have solved the problem, since with $v_{r,f} = 0$ we have the final velocities

$$v_{1,f} = v_{2,f} = \dot{X} \quad (2.30)$$

Not that the velocity of the c.o.m. follows from conservation of total linear momentum, which follows from Newton's third law and does not depend on forces being conservative.

To come to the same conclusion strictly using Hamilton's equations of motion, we could extend

the model by including internal degrees of freedom in the colliding objects, so that the relative kinetic energy can be converted to internal motion that represents heating of the objects due to the collision.

2.3 Center-of-mass frame

We solved the collision problem using the **lab-frame coordinates** (x_1, x_2) and the **generalized coordinates** (X, r). We found that the internal motion is completely **decoupled** from the c.o.m. motion. For this reason, it can be convenient to introduce a new frame, **the center-of-mass frame**, which lets us focus on the internal motion. In this frame, the c.o.m. is taken as the origin of the frame. In this frame, the coordinates of the particles are $(\tilde{x}_1, \tilde{x}_2)$, with

$$\tilde{x}_i \equiv x_i - X. \tag{2.31}$$

Since there is only one degree of freedom for the internal motion, these two coordinates must be **redundant**. From Eq. (2.2) we find

$$\tilde{x}_1 = -\frac{m_1}{m_1 + m_2} r \tag{2.32}$$

$$\tilde{x}_2 = \frac{m_2}{m_1 + m_2} r, \tag{2.33}$$

and from taking the time derivative we find the velocities

$$\tilde{v}_1 = v_1 - \dot{X} = -\frac{m_1}{m_1 + m_2} v_r \tag{2.34}$$

$$\tilde{v}_2 = v_2 - \dot{X} = \frac{m_2}{m_1 + m_2} v_r. \tag{2.35}$$

Thus, we may verify that in this new frame the c.o.m. is

$$\tilde{X} = m_1 \tilde{x}_1 + m_2 \tilde{x}_2 = 0 \tag{2.36}$$

and its velocity is zero,

$$\frac{d}{dt} \tilde{X} = 0. \tag{2.37}$$

The relative coordinate is still

$$r = x_2 - x_1 = \tilde{x}_2 - \tilde{x}_1, \tag{2.38}$$

so after converting the initial velocities (v_1, v_2) to the new frame, $(\tilde{v}_1, \tilde{v}_2)$, we study the collision in this new frame, where the c.o.m. motion is zero, and the internal Hamiltonian $H_r(r, p_r)$ describes the system.

The c.o.m. frame here is an example of a **inertial frame**, which may be defined as a frame in which Newton's laws hold.

2.4 Collisions in 2D

To describe collisions of two particles in 2D, we use vector notation, with the positions of the particles given by $\boldsymbol{r}_1$ and $\boldsymbol{r}_2$. Thus, in 2D, we have four degrees of freedom. We switch to generalized coordinates $(\boldsymbol{X}, \boldsymbol{r})$, with $\boldsymbol{X}$ the center of mass and $\boldsymbol{r} = \boldsymbol{r}_2 - \boldsymbol{r}_1$ the relative coordinate. To derive the conjugate momenta we simply repeat the above derivation for the x and y coordinates. For the potential, $V(r)$, we still assume that it only depends on the distance between the particles, but now $r = |\boldsymbol{r}|$ (instead of $x_2 - x_1$). The Hamiltonian,

$$H(\boldsymbol{X}, \boldsymbol{P}, \boldsymbol{r}, \boldsymbol{p}) = \frac{P^2}{2M} + \frac{p_r^2}{2\mu} + V(r), \tag{2.39}$$

looks exactly like the 1D case, but we must remember that now

$$P^2 = \boldsymbol{P} \cdot \boldsymbol{P} = P_x^2 + P_y^2 \tag{2.40}$$

$$p_r^2 = \boldsymbol{p}_r \cdot \boldsymbol{p}_r = p_x^2 + p_y^2 \tag{2.41}$$

with relative momentum

$$\boldsymbol{p}_r = \mu(\boldsymbol{v}_2 - \boldsymbol{v}_1) \tag{2.42}$$

and total linear momentum

$$\boldsymbol{P} = \boldsymbol{p}_1 + \boldsymbol{p}_2 = m_1\boldsymbol{v}_1 + m_2\boldsymbol{v}_2. \tag{2.43}$$

The c.o.m. motion is again linear with constant velocity, so in vector notation

$$\boldsymbol{X}(t) = \boldsymbol{X}(0) + \frac{\boldsymbol{P}}{M}t. \tag{2.44}$$

For elastic collisions we have conservation of energy (E) for the internal motion

$$\frac{p_r^2}{2\mu} = E. \tag{2.45}$$

Thus, energy conservation only gives us the magnitude of the final momentum, **but not its direction**,

$$p_{r,f}^2 = p_{x,f}^2 + p_{y,f}^2 = 2\mu E. \tag{2.46}$$

and the final relative velocity is

$$v_{r,f} = \frac{p_{r,f}}{\mu}. \tag{2.47}$$

To fully solve the problem we would need to know the exact potential $V(r)$, and we would have to solve the internal equations of motion for $\boldsymbol{r}$.

However, in an experiment we could detect only particles moving in a certain direction. Let's say the detector is sensitive to particle 2 moving in direction

$$\hat{\boldsymbol{d}} = \begin{pmatrix}\cos\phi \\ \sin\phi\end{pmatrix}, \tag{2.48}$$

where ϕ is given and the hat indicates that the vector is normalized. Thus, the lab-frame velocity of particle 2 is

$$\boldsymbol{v}_2 = v_{2,f}\hat{\boldsymbol{d}}. \tag{2.49}$$

So we want to solve $v_{2,f}$, and what we know from solving the elastic scattering problem is the magnitude of the relative velocity, $v_{r,f}$. To do this, we first note that in the c.o.m. we have

$$\tilde{\boldsymbol{v}}_2 = v_{2,f}\hat{\boldsymbol{d}} - \dot{X}, \tag{2.50}$$

where we know $\dot{\boldsymbol{X}}$ from the initial conditions and conservation of total linear momentum. Since in the c.o.m. frame the total linear momentum is zero, we can relate the velocity of particle 1 to that of 2

$$\tilde{\boldsymbol{v}}_1 = -\frac{m_2}{m_1}\tilde{\boldsymbol{v}}_2. \tag{2.51}$$

Thus, the relative velocity is a function of $v_{2,f}$,

$$\begin{aligned}\boldsymbol{v}_r &= \tilde{\boldsymbol{v}}_2 - \tilde{\boldsymbol{v}}_1 \\ &= \left(1 + \frac{m_2}{m_1}\right)(v_{2,f}\hat{\boldsymbol{d}} - \dot{\boldsymbol{X}}).\end{aligned} \tag{2.52}$$

Since we know the length of vector $\boldsymbol{v}_r$ we found a quadratic equation for $v_{2,f}$

$$v_{r,f}^2 = \left(1 + \frac{m_2}{m_1}\right)^2 |v_{2,f}\hat{\boldsymbol{d}} - \dot{\boldsymbol{X}}|^2. \tag{2.53}$$

Since we only used energy conservation, which also hold if the interaction potential is zero, we know that one solution corresponds the velocities being equal to the initial condition, and so the other solution must correspond to the elastic scattering event.

2.5 Inelastic collisions in 2D

In a fully inelastic collision the internal energy E is set to zero as before, and after the collision the particles move with the center of mass.

If one of the particles is a molecule that gets rotationally of vibrationally excited, we can still

use the calculation that we used for elastic collisions, except that we must reduce the internal energy E by the energy absorbed by the molecule.

2.6 Collisions in 3D

In this case we have a problem with six degrees of freedom. Using total linear momentum and energy conservation leaves us with 6-3-1=2 unknowns. The center of mass will still move linearly with constant velocity and after the collision the particles will move away with a speed that we compute from energy conservation. There are still two degrees of freedom in the direction the particles are moving in the c.o.m. frame, so after the collision, the particles will be moving on a linearly expanding sphere with the c.o.m. as its origin.

Later, we will see that conservation of angular momentum forces the motion to be in a plane, so after the collision particles will be on a circle and there is only one unknown angle giving the direction. Note that in a crossed beam experiment with perfect control over velocities, one has no control over the plane in which the collision partners move, so collision products will still be found on the so called "Newton sphere".

Chapter 3

Rotational motion in 2D

Polar coordinates (r, ϕ) are particularly convenient generalized coordinates to describe rotation in a plane. They are related to Cartesian coordinates by

$$x = r\cos\phi \tag{3.1}$$
$$y = r\sin\phi. \tag{3.2}$$

We will now follow the general approach of Hamiltonian mechanics to derive the equations of motion for these coordinates. First, we write down the kinetic energy in terms of velocities,

$$v_x = \dot{x} = \dot{r}\cos\phi - r\dot{\phi}\sin\phi \tag{3.3}$$
$$v_y = \dot{y} = \dot{r}\sin\phi + r\dot{\phi}\cos\phi. \tag{3.4}$$

Expressed in generalized coordinates we find

$$T(r, \dot{r}, \dot{\phi}) = \frac{1}{2}m\dot{r}^2 + \frac{1}{2}mr^2\dot{\phi}^2. \tag{3.5}$$

The result is relatively simple because we could use $\cos^2\phi + \sin^2\phi = 1$ and the cross terms with $\dot{r}\dot{\phi}$ that we get from v_x^2 and v_y^2 cancel each other.

For the conjugate momenta we find

$$p_r = \frac{\partial}{\partial\dot{r}}T = m\dot{r} \tag{3.6}$$
$$p_\phi = \frac{\partial}{\partial\dot{\phi}}T = mr^2\dot{\phi}. \tag{3.7}$$

The Hamiltonian is

$$H(r, p_r, \phi, p_\phi) = \frac{p_r^2}{2m} + \frac{\dot{\phi}^2}{2mr^2} + V(r, \phi). \tag{3.8}$$

It is conventional to denote the **angular velocity** as

$$\omega \equiv \dot{\phi}. \tag{3.9}$$

The momentum conjugate to the angle ϕ is called **angular momentum**, and it is conventionally denoted as

$$L \equiv p_\phi. \tag{3.10}$$

Furthermore, the **moment of inertia** is defined by

$$I(r) \equiv mr^2. \tag{3.11}$$

Thus, for the angular momentum L we have

$$L = I(r)\omega \tag{3.12}$$

and the Hamiltonian becomes

$$H = \frac{p_r^2}{2m} + \frac{L^2}{2I(r)} + V(r, \phi). \tag{3.13}$$

The Hamiltonian equations of motion are

$$\dot{r} = \frac{\partial H}{\partial p_r} = \frac{p_r}{m} \tag{3.14}$$

$$\dot{p_r} = -\frac{\partial H}{\partial r} = -\frac{\partial}{\partial r}\left[\frac{L^2}{2I(r)} + V(r,\phi)\right] \tag{3.15}$$

$$\omega = \frac{\partial H}{\partial L} = \frac{L}{I(r)} \tag{3.16}$$

$$\dot{L} = -\frac{\partial H}{\partial \phi} = -\frac{\partial}{\partial \phi} V(r,\phi) \tag{3.17}$$

For the motion of a projectile under the force of gravity, where the potential depends on $y = r\sin\phi$, we see that with these new coordinates the potential will actually depend of both r and ϕ, so the Hamiltonian does not separate, and we have two coupled degrees of freedom. In the following, we will consider several cases where polar coordinates have a big advantage over Cartesian coordinates.

3.0.1 Circular motion

First, consider the constraint motion, where the distance r is fixed, so the particle moves in a circle. In Hamiltonian mechanics we can simply drop the kinetic energy term associated with the constraint, so the Hamiltonian will be

$$H = \frac{L^2}{2I(r)} + V(r,\phi) \tag{3.18}$$

For a potential that is actually independent of ϕ we know from Hamilton's equation of motion that the angular momentum L is conserved. This is again an example of Noether's theorem, where the continuous symmetry **orientation**, i.e., the invariance of the Hamiltonian under changes of ϕ lead to a conserved quantity, **angular momentum**. With L, and hence the angular velocity ω = fixed, the time-dependent orientation is

$$\phi(t) = \phi(0) + \omega t = \phi(0) + \frac{L}{I(r)}t. \tag{3.19}$$

Note that unlike in Newtonian mechanics, we do not have to think about the force that is required to make the particle move in a circle. However, since after solving for the time-dependent angle $\phi(t)$, we can put it back into Eqs. (3.1) and (3.2), we can compute the acceleration, and get the force using Newton's second law. With $\dot{r} = 0$, and constant angular velocity, the velocities are

$$v_x = -r\omega\sin\phi \tag{3.20}$$

$$v_y = r\omega\cos\phi \tag{3.21}$$

so the acceleration is

$$a_x = r\omega^2\cos\phi \tag{3.22}$$

$$a_y = -r\omega^2\sin\phi \tag{3.23}$$

or in vector notation

$$\boldsymbol{a} = \ddot{\boldsymbol{r}} = -\omega^2\boldsymbol{r}. \tag{3.24}$$

So the so-called **centripetal force** ("center seeking") is thus

$$\boldsymbol{F}_{\rm c} = m\boldsymbol{a} = -m\omega^2\boldsymbol{r}. \tag{3.25}$$

This **centripetal force** would be minus the derivative of the radial potential that keeps r fixed, e.g., it could be the result of the tension in a string tied to the particle and the center of rotation. Since this force derives from a potential, it is a **real force**.

The **centrifugal force** ("center-fleeing") is a **fictitious** force that has the same magnitude as the centripetal force, but opposite sign. It is the outward pulling force you would feel as a result of the rotational motion.

3.0.2 Spinning ring

If we have N particles with masses m_i, all making a circular motion around the same point, with the same radius, and with the same angular velocity ω, but possibly different $\phi_i(t=0)$, the kinetic energy is

$$T(r,\omega) = \frac{1}{2}\sum_i m_i r^2\omega^2 = \frac{1}{2}Mr^2\omega^2, \quad (3.26)$$

where M is the total mass of the spinning ring

$$M = \sum_i m_i. \quad (3.27)$$

If the relative positions of the masses on the ring are fixed, the orientation of the disc still depends on a single angle ϕ, so the Hamiltonian of Eq. (3.18) still applies, except that the moment of inertia is given by

$$I(r) = Mr^2. \quad (3.28)$$

We still have $L = I\omega$, and if the potential is independent of ϕ, the angular momentum is again conserved and Eq. (3.19) still applies.

3.0.3 Rigid rotor

For a spinning rigid object, again, the only change required is to re-compute the moment of inertia. If we model a rigid object as a set of point particles with masses m_i, and at distances r_i to the rotation center, but all rotating with the same angular velocity ω, the moment of inertia becomes

$$I = \sum_i m_i r_i^2. \quad (3.29)$$

We can also model a spinning disc with a fixed density per area (ρ). In this case, the mass of the material at a distance to the rotation axis in the interval $[r, r+dr]$, for small dr is

$$dM = \rho 2\pi r dr \quad (3.30)$$

and its contribution to the moment of inertia is

$$dI = r^2 dM \quad (3.31)$$

For a disc with radius r_0 we find the total moment of inertia by integration

$$I_{\text{disc}}(r_0) = \int_0^{r_0} 2\pi r^3 dr = \frac{1}{2}\rho\pi r_0^4. \quad (3.32)$$

Since the area of the disc is $A = \pi r_0^2$ and its mass is $M = \rho A$, we have

$$I_{\text{disc}}(r_0) = \frac{1}{2}Mr_0^2 \quad (3.33)$$

This expression also applies to the moment of inertial of a solid cylinder made of a single material, assuming it rotates around it center axis.

Bibliography

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