Lecture Notes in Classical Mechanics (80751)

Raz Kupferman
Institute of Mathematics
The Hebrew University

July 14, 2008

Contents

Chapter 1

Preliminaries

1.1 Vector calculus

According to classical physics, "reality" takes place in a product space $\mathbb{R}^3 \times \mathbb{R}$, where $\mathbb{R}^3$ represents ***space*** and $\mathbb{R}$ represents ***time***. The notions of space and time are axiomatic in classical physics, meaning that they do not deserve a definition. (In ***relativistic physics***, the notions of space and time are intermingled, and one rather speaks about a four dimensional ***space-time***.)

Because the physical space is a three-dimensional vector space, we will have to deal extensively with vectors in $\mathbb{R}^3$. We will denote vectors by boldface characters, e.g., $\mathbf{a}, \mathbf{b}, \mathbf{c}$. After choosing an an orthonormal basis, the entries, or ***components*** of a vector in $\mathbb{R}^3$ are commonly denoted by

$$\mathbf{a} = (a_1, a_2, a_3).$$

At times we will use different notations, such as $\mathbf{r} = (x, y, z)$.

Let $\mathbf{a}$ and $\mathbf{b}$ be two vectors in $\mathbb{R}^3$. Their ***scalar product***, or ***dot product*** is a real number defined by

$$\mathbf{a} \cdot \mathbf{b} = a_1 b_1 + a_2 b_2 + a_3 b_3 = \sum_{i=1}^{3} a_i b_i.$$

Physicists often adopt a notational convention, the ***Einstein summation convention***, whereby indexes that appear twice in an expression are summed over, without need of the summation sign. That is,

$$\mathbf{a} \cdot \mathbf{b} = a_i b_i.$$

While confusing at first, this notation ends up being very useful. Of course, what physicists call a scalar product is nothing but the standard ***inner product*** in $\mathbb{R}^3$.

The ***length***, or ***magnitude*** of a vector $\mathbf{a}$, is its ***Euclidean norm***,

$$|\mathbf{a}| = (\mathbf{a}\cdot\mathbf{a})^{1/2} = \sqrt{a_i a_i}.$$

The scalar product of two vectors, can be attributed a geometric meaning that involves the angle, θ, between the two vectors,

$$\mathbf{a}\cdot\mathbf{b} = |\mathbf{a}||\mathbf{b}|\cos\theta.$$

Two (non-zero) vectors are said to be ***orthogonal*** (denoted $\mathbf{a} \perp \mathbf{b}$) if their dot product vanishes, i.e., if $\theta = \pm\pi/2$.

We will often denote the standard basis in $\mathbb{R}^3$ by

$$\mathbf{e}_1 = (1,0,0), \qquad \mathbf{e}_2 = (0,1,0), \qquad \text{and} \qquad \mathbf{e}_3 = (0,0,1).$$

Thus, a vector can be also written as

$$\mathbf{a} = a_1\mathbf{e}_1 + a_2\mathbf{e}_2 + a_3\mathbf{e}_3 = a_i\mathbf{e}_i.$$

Other times, we will rather denote $\mathbf{e}_1 = \hat{\mathbf{x}}$, $\mathbf{e}_2 = \hat{\mathbf{y}}$, and $\mathbf{e}_3 = \hat{\mathbf{z}}$.

Proposition 1.1 The dot product satisfies the following properties:

① *It is commutative,* $\mathbf{a}\cdot\mathbf{b} = \mathbf{b}\cdot\mathbf{a}$.
② *It is bilinear,* $(\alpha\mathbf{a})\cdot\mathbf{b} = \alpha(\mathbf{a}\cdot\mathbf{b})$.
③ *It is distributive,* $\mathbf{a}\cdot(\mathbf{b}+\mathbf{c}) = \mathbf{a}\cdot\mathbf{b} + \mathbf{a}\cdot\mathbf{c}$.
④ *The Cauchy-Schwarz inequality,* $|\mathbf{a}\cdot\mathbf{b}| \leq |\mathbf{a}|\,|\mathbf{b}|$.

We define another product between pairs of vectors, the ***cross product***, or the ***vector product***. Unlike the dot product, the cross product results in a vector. It can be defined in several ways, for example,

$$\mathbf{a}\times\mathbf{b} = \begin{vmatrix} \mathbf{e}_1 & \mathbf{e}_2 & \mathbf{e}_3 \\ a_1 & a_2 & a_3 \\ b_1 & b_2 & b_3 \end{vmatrix} = (a_2b_3 - a_3b_2)\mathbf{e}_1 + (a_3b_1 - a_1b_3)\mathbf{e}_2 + (a_1b_2 - a_2b_1)\mathbf{e}_3.$$

The other way is to define the cross products of all pairs of basis vectors, e.g.,

$$\mathbf{e}_1\times\mathbf{e}_1 = 0, \qquad \mathbf{e}_1\times\mathbf{e}_2 = \mathbf{e}_3, \quad \text{etc.},$$

and impose bilinearity and distributivity. A third definition introduces the ***Levi-Civita tensor***,

$$\epsilon_{ijk} = \begin{cases} +1 & \text{if } (i,j,k) \text{ is } (1,2,3), (2,3,1), \text{ or } (3,1,2) \\ -1 & \text{if } (i,j,k) \text{ is } (1,3,2), (2,1,3), \text{ or } (3,2,1) \\ 0 & \text{otherwise.} \end{cases}.$$

Then, the cross product takes the simple form,

$$\mathbf{a} \times \mathbf{b} = \epsilon_{ijk} \mathbf{e}_i a_j b_k.$$

A very useful property of the Levi-Civita tensor (easily checked by explicit substitution) is

$$\epsilon_{ijk}\epsilon_{imn} = \delta_{jm}\delta_{kn} - \delta_{jn}\delta_{km}. \tag{1.1}$$

The cross product also has a geometric interpretation. First, we claim that for every $\mathbf{a}, \mathbf{b}$,

$$\mathbf{a} \cdot (\mathbf{a} \times \mathbf{b}) = \mathbf{b} \cdot (\mathbf{a} \times \mathbf{b}) = 0,$$

that is, the cross product of two vectors is perpendicular to both. While this can be verified by a (relatively) tedious substitution, the clean way of deriving this result is using our index notation, e.g.,

$$\mathbf{a} \cdot (\mathbf{a} \times \mathbf{b}) = (a_i)(\epsilon_{ikl} a_k b_l) = \epsilon_{ikl} a_i a_k b_l.$$

Now, ϵ_{ikl} changes sign when a pair of indexes is switched, hence,

$$\mathbf{a} \cdot (\mathbf{a} \times \mathbf{b}) = -\epsilon_{kil} a_i a_k b_l = -\epsilon_{ikl} a_i a_k b_l,$$

where we have just renamed the summation indexes $i \to k$ and $k \to i$. Thus, this triple product equals minus itself, hence it is zero.

What about its magnitude? Note that

$$|\mathbf{a} \times \mathbf{b}|^2 = (\mathbf{a} \times \mathbf{b}) \cdot (\mathbf{a} \times \mathbf{b}) = \epsilon_{ijk} a_j b_k \epsilon_{imn} a_m b_n.$$

Using the product formula (1.1) for the Levi-Civita tensor,

$$\begin{aligned} |\mathbf{a} \times \mathbf{b}|^2 &= (\delta_{jm}\delta_{kn} - \delta_{jn}\delta_{km}) a_j b_k a_m b_n \\ &= a_j b_k a_j b_k - a_j b_k a_k b_j = |\mathbf{a}|^2 |\mathbf{b}|^2 - (\mathbf{a} \cdot \mathbf{b})^2 = |\mathbf{a}|^2 |\mathbf{b}|^2 (1 - \cos^2\theta), \end{aligned}$$

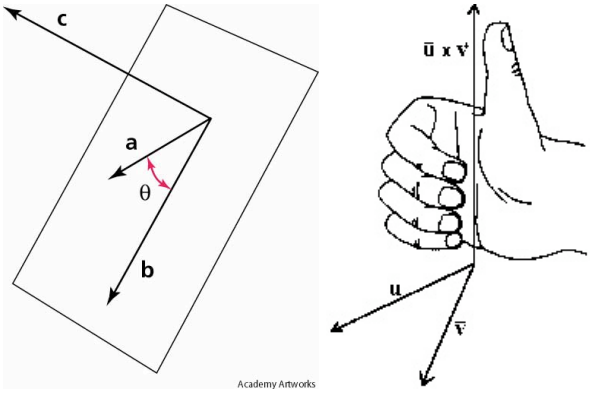


Figure 1.1: Visualization of the cross product.

i.e.,

$$|\mathbf{a} \times \mathbf{b}| = |\mathbf{a}||\mathbf{b}| \sin\theta.$$

Thus, the cross product of two vectors is a vector perpendicular to both, whose magnitude equals to the area of the parallelepiped formed by the two vectors. Its direction is determined by the ***right hand rule*** (see Figure 1.1).

Proposition 1.2 *The cross product satisfies the following algebraic properties:*

① *Anti-symmetry:* $\mathbf{a} \times \mathbf{b} = -\mathbf{b} \times \mathbf{a}$.

② *Distributivity:* $\mathbf{a} \times (\mathbf{b} + \mathbf{c}) = \mathbf{a} \times \mathbf{b} + \mathbf{a} \times \mathbf{c}$.

③ *Bilinearity,* $(\alpha\mathbf{a}) \times \mathbf{b} = \alpha(\mathbf{a} \times \mathbf{b})$.

④ *It is not associative.*

⑤ *Jacobi's identity:* $\mathbf{a} \times (\mathbf{b} \times \mathbf{c}) + \mathbf{c} \times (\mathbf{a} \times \mathbf{b}) + \mathbf{b} \times (\mathbf{c} \times \mathbf{a}) = 0$.

⑥ *The vector triple product, or "BAC minus CAB" formula:* $\mathbf{a} \times (\mathbf{b} \times \mathbf{c}) = \mathbf{b}(\mathbf{a} \cdot \mathbf{c}) - \mathbf{c}(\mathbf{a} \cdot \mathbf{b})$.

⑦ *The scalar triple product formula,* $\mathbf{a} \cdot (\mathbf{b} \times \mathbf{c}) = \mathbf{b} \cdot (\mathbf{c} \times \mathbf{a}) = \mathbf{c} \cdot (\mathbf{a} \times \mathbf{b})$.

✎ *Exercise 1.1* Prove it.

1.2 Dimensional analysis

Units of measurement All physical quantities are expressed in terms of ***numbers***, obtained through ***measurements***, during which comparison is made with a ***standard***, or, a ***unit of measurement***. For example, the length of a ruler is measured by comparison to a standard, say the meter; the mass of a rock is measured by comparison with a unit mass, say, the gram; the duration of the day is measured by comparison with a unit time, say the time it takes a standard hour-glass to empty; the (mean) velocity of a car is measured by measuring the distance it went, say in inches, the time it took, say in milliseconds, and dividing those two numbers.

Fundamental and derived units The units of measurements are divided into two categories: ***fundamental units*** and ***derived units***. Suppose we want to study a class of phenomena, for example, the motion of bodies. We may list all the quantities which will ever be measured, and for certain of them choose units of measurement, which we will call fundamental units; the choice is arbitrary. For example, we may choose fundamental units of mass, length, and time (but also force, length and time). Derived units of measurements are based upon the fundamental units via some method of measurement (perhaps only conceptual). For example, the measurement of velocity, whose (derived) units uses the (fundamental) units of length and time.

Systems of units A set of fundamental units that is *sufficient* for measuring the properties of a class of phenomena is called a ***system of units***, for example,

cgs = centimeter, gram, second

in mechanics.

Classes of systems of units Two systems of units which differ only in the magnitude of their standards, but not in their physical natures, are said to belong to the same class. For example, all systems of units which are of the form

unit of length = cm/L
unit of mass = gram/M
unit of time = second/T,

with $L, M, T > 0$, belong to the same class (the LMT class). Another class, the LFT class consists of systems of units of the form

unit of length = cm/L
unit of force = kg-f/F
unit of time = second/T.

(For the time being, ignore the fact we have no clue what "force" means. All you need to understand, is that it is a physical quantity that can be measured with the appropriate apparatus.)

Note, however, that while both classes, the LMT and LFT classes, form a system of units for a class of physical phenomena which we call mechanics, they are not a sufficient set of units if we want, in addition, to measure, say, temperature, or an electric charge.

Dimensions Suppose we choose a class of system of units, for example, the LMT class in mechanics, and suppose we change our system of units within the same class, by decreasing the length unit by a factor L, the mass unit by a factor M, and the time unit by a factor T (e.g., we use centimeters rather than meters, ounces rather than grams, and weeks rather than seconds). How will this affect the magnitude of the outcome of measurements?

Length measurements will be magnified by a factor of L; mass measurements will be magnified by a factor of M; time measurements will be magnified by a factor of T; velocity measurements will be magnified by a factor of LT^{-1}, and so on. Every physical quantity will be magnified by a factor which depends on L, M, T. That is, every physical quantity has an associated function of L, M, T, which we call its ***dimension***. The dimension of mass density (mass per unit volume), for example, is ML^{-3}. A quantity which remains invariant under a change of units is called ***dimensionless***, and its dimension is by definition one. Note that *the dimension of a physical quantity depends on the class of the system of units!*

✎ *Exercise 1.2* Consider the MVT class where the fundamental units are that of mass, velocity and time. What kind of experiment measures length? What is the dimension of length? What is the dimension of mass density?

Physics is usually not thought in terms of an axiomatic theory. One rather speaks about ***fundamental principles***. The most fundamental principle in all branches of physics is probably the following:

The laws of physics are invariant under the choice of systems of units.

What are ***laws of physics***? They are relations between measurable quantities. For example, a physical law states that the force of attraction between two physical bodies (which can be measured) is proportional to the masses of each of them (which can be measured), and inversely proportional to the square of their separation (which can be measured independently).

The first observation to be made is that if a physical law is of the form

$$\text{expression 1} = \text{expression 2},$$

then both expression must have the same dimension, otherwise the identity could not hold independently on the system of units.

The dimension is always a power-law monomial So far, all dimension functions were always power-law monomials. Is it a coincidence? Suppose we work within the LMT class, and we are interested in some quantity a. By assumption (that the LMT class is complete), the dimension of a only depends on L, M, T:

$$[a] = f(L, M, T).$$

What does it mean? That if we change units by dividing the units of length, mass and time by L_1, M_1, T_1, the measured value a_1 will increase by $f(L_1, M_1, T_1)$. Similarly, if we change units by dividing the units of length, mass and time by L_2, M_2, T_2, the measured value a_2 will increase by $f(L_2, M_2, T_2)$. That is,

$$\frac{a_2}{a_1} = \frac{f(L_2, M_2, T_2)}{f(L_1, M_1, T_1)}.$$

The underlying assumption is that all systems of units within a given class are equivalent. Thus, we may think of the system 1 as the original system, and system 2 as obtained by decreasing the fundamental units by L_2/L_1, M_2/M_1, and T_2/T_1. Then,

$$a_2 = a_1\, f(L_2/L_1, M_2/M_1, T_2/T_1),$$

from which immediately follows the *functional equation*

$$\frac{f(L_2, M_2, T_2)}{f(L_1, M_1, T_1)} = f\left(\frac{L_2}{L_1}, \frac{M_2}{M_1}, \frac{T_2}{T_1}\right).$$

What can be learned from such a functional relation?

Assuming that the dimension function is smooth, we differentiate both sides with respect to L_2 and set $L_2 = L_1 = L$, $M_2 = M_1 = M$, and $T_2 = T_1 = T$,

$$\frac{1}{f(L,M,T)}\frac{\partial f}{\partial L}(L,M,T) = \frac{1}{L}\frac{\partial f}{\partial L}(1,1,1) \equiv \frac{\alpha}{L},$$

from which we conclude that

$$f(L,M,T) = L^{\alpha} g(M,T).$$

Substituting into the functional equation we get

$$\frac{g(M_2,T_2)}{g(M_1,T_1)} = g\left(\frac{M_2}{M_1}, \frac{T_2}{T_1}\right),$$

and by the same procedure get that

$$g(M,T) = M^{\beta} h(T).$$

Repeating this for a third time we get $h(T) = cT^{\gamma}$, i.e.,

$$f(L,M,T) = c\, L^{\alpha} M^{\beta} T^{\gamma}.$$

Since $f(1,1,1) = 1$, we conclude that $c = 1$.

Quantities with independent dimensions The physical quantities $a_1, \ldots, a_k$ are said to have ***independent dimensions*** if none of these quantities have a dimension which can be presented as a power monomial of the dimensions of the remaining quantities. It is perhaps easier to give a logarithmic formulation. In the LMT system, for example, every set of physical quantities (a_i), $i = 1, \ldots, k$, has a dimension functions of the form,

$$\begin{aligned} \log[a_1] &= \alpha_1 \log L + \beta_1 \log M + \gamma_1 \log T \\ \vdots \quad &= \quad \vdots \\ \log[a_k] &= \alpha_k \log L + \beta_k \log M + \gamma_k \log T \end{aligned}$$

That is, the logarithms of dimensions form a vector space with basis vectors $\log L$, $\log M$, $\log T$. Independence of dimension is linear independence over this space.

Obviously, in this case there can be at most three physical quantities of independent dimension.

Suppose now physical quantities $a_1, \ldots, a_k$ and $b_1, \ldots, b_m$, such that the first k have independent dimensions, and all the m additional quantities have dimensions that depend on the dimensions of the first k quantities. The fact that the a_i have independent dimensions implies that if we work, say, with an $L_1 L_2 \ldots L_r$ system, then necessarily, $r \geq k$ and if

$$\begin{pmatrix} \log [a_1] \\ \vdots \\ \log [a_k] \end{pmatrix} = \begin{pmatrix} \gamma_{11} & \cdots & \gamma_{1r} \\ \vdots & \vdots & \vdots \\ \gamma_{k1} & \cdots & \gamma_{kr} \end{pmatrix} \begin{pmatrix} \log L_1 \\ \vdots \\ \log L_r \end{pmatrix},$$

then the matrix of coefficients has full rank (i.e., k). This has an important implication: it is possible to change units of measurement such that, as a result, a single a_j changes its value, while all the other remain fixed.

Now we come to the b_j. Since their dimensions depend on the dimensions of the a_j, then there exist constants α_{ij}, such that

$$\begin{aligned} \log [b_1] &= \alpha_{11} \log [a_1] + \cdots + \alpha_{1k} \log [a_k] \\ \vdots \quad &= \quad \vdots \\ \log [b_m] &= \alpha_{m1} \log [a_1] + \cdots + \alpha_{mk} \log [a_k] . \end{aligned}$$

Consider now the following new quantities,

$$\begin{aligned} \Pi_1 &= \frac{b_1}{a_1^{\alpha_{11}} \ldots a_k^{\alpha_{1k}}} \\ \vdots &= \quad \vdots \\ \Pi_m &= \frac{b_m}{a_1^{\alpha_{m1}} \ldots a_k^{\alpha_{mk}}}. \end{aligned}$$

It is easy to see that these quantities are dimensionless; their value does not change, no matter how we change our units of measurement.

Physical laws A physical law always consists of a relationship between physical quantities,

$$c = f(a_1, \ldots, a_k, b_1, \ldots, b_m). \tag{1.2}$$

Here c is the quantity being determined and $a_1, \ldots, a_k, b_1, \ldots, b_m$ are all the quantities it depends upon (as above, the a_j have independent dimensions). It is important to stress that a physical law is an equation that relates between measurable quantities. There exists a function f, such that if one measures the quantities a_j, b_j, and c, the *numbers* thus obtained satisfy the prescribed equation.

We first claim that the dimension of c must depend on the dimension of the a_j. Why is it so? Otherwise, we could perform a change of units of measurement, such that the value of c changes, while the values of all the a_j (and consequently all the b_j) remain unchanged. This would contradict the assumption that f is only a function of those physical quantities. Thus, there exist numbers $\beta_1, \ldots, \beta_k$, such that

$$[c] = [a_1]^{\beta_1} \ldots [a_k]^{\beta_k},$$

and the physical quantity

$$\Pi = \frac{c}{a_1^{\beta_1} \ldots a_k^{\beta_k}}$$

is dimensionless.

The Π theorem Using our definitions of dimensionless quantities, we can rewrite (1.2) as follows:

$$\Pi = \frac{1}{a_1^{\beta_1} \ldots a_k^{\beta_k}} f\left(a_1, \ldots, a_k, a_1^{\alpha_{11}} \ldots a_k^{\alpha_{1k}} \Pi_1, \ldots, a_1^{\alpha_{m1}} \ldots a_k^{\alpha_{mk}} \Pi_m\right),$$

and this can be brought into an alternative form,

$$\Pi = \mathcal{F}(a_1, \ldots, a_k, \Pi_1, \ldots, \Pi_m).$$

That is, we rewrote (1.2) as a relation between k physical quantities of independent dimension and m dimensionless quantities, on one side, and a dimensionless quantity, on the other side.

Now remember we can perform a change of units such that only a_1 changes its value. Thus, $\mathcal{F}$ cannot depend on a_1. By repeating this argument k times we end up with the conclusion that

$$\Pi = \mathcal{F}(\Pi_1, \ldots, \Pi_m).$$

This is known as the "Π-theorem". *A physical relationship between some dimensional parameter and several dimensional governing parameters can be rewritten*

as a relation between some dimensionless parameter and several dimensionless products of the governing parameters.

What is the immediate gain? A law that seemed to depend on $k + m$ parameters reduces into a law that only depends on m parameters. This might be a huge reduction.

Example: In Euclidean geometry it is known that the area S of a right triangle depends only on the length of its hypotenuse, c, and the magnitude ϕ of, say, the smaller of its acute angles. Thus,

$$S = f(c, \phi).$$

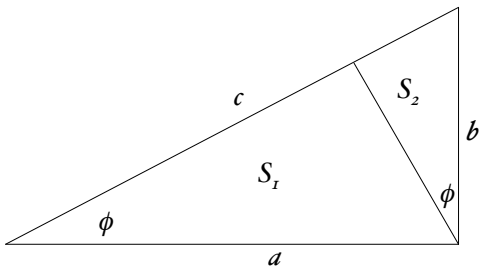
For this problem we can do well with for only fundamental units those of length (an L system). In this case, c has dimension L, ϕ is dimensionless and S has dimension L^2. By the Π-theorem, the dimensionless quantity $\Pi = S/c^2$ can only depend on the dimensionless parameter $\Pi_1 = \phi$,

$$\Pi = \mathcal{F}(\Pi_1) \qquad \Rightarrow \qquad S = c^2\,\mathcal{F}(\phi).$$

Without caring what the function $\mathcal{F}$ actually is, we have at once,

$$S_1 = a^2\,\mathcal{F}(\phi), \qquad S_2 = b^2\,\mathcal{F}(\phi), \qquad S_1 + S^2 = c^2\,\mathcal{F}(\phi),$$

from which follows Pythagoras' theorem.



▲

Example: A mass m is thrown vertically with velocity v. What is the maximal height h it will attain? We start with

$$h = f(m, v, g).$$

Since $[h] = L$, $[m] = M$, $[v] = L/T$ and $[g] = L/T^2$, we conclude from the Π-theorem that

$$\Pi = \frac{h}{\sqrt{v^2/g}} = \text{const.}$$

▲

✎ *Exercise 1.3* A pendulum is a massive particle suspended on a string (which we assume to have negligible mass). If one perturbs the pendulum (for example by placing it at the equilibrium point, but assigning it an initial velocity), then the pendulum performs a periodic motion. Suppose we want to find a law to predict the period, τ, of the motion. We start by making a list of all quantities that τ may depend upon: (1) the mass m of of the particle, (2) the initial velocity v, (3) earth's acceleration g, and (4) the length of the string, ℓ. In the LMT system we have

$$[\tau] = T \quad [m] = M \quad [v] = \frac{L}{T} \quad [g] = \frac{L}{T^2} \quad [\ell] = L.$$

① What can you say about the function

$$\tau = f(m, v, g, \ell)$$

based on dimensional analysis?

② Suppose now an experimentalist tells you that the period does not depend on the initial velocity. How will your answer change?

Example: In an atomic explosion, a large amount of energy E is released within a small region, and a strong spherical shock wave develops at the point of detonation. In the early stages, the pressure behind the shock wave is huge compared to the atmospheric pressure, which is completely negligible. If r denotes the radius of the wave and t is time, the radius is only expected to depend on

$$r = f(t, E, \rho),$$

where ρ is the density of the air at equilibrium (no shock wave without air density, and other characteristics of air, such as sound wave speed are irrelevant for shock waves).

The dimensions of the governing parameters in the LMT class are

$$[t] = T \qquad [E] = ML^2T^{-2} \qquad [\rho] = ML^{-3}.$$

It is easy to see that those are all independent, i.e., $k = 3$ and $m = 0$. The dimension of r is L, so that

$$\Pi = \frac{\rho^{1/5}\, r}{E^{1/5} t^{2/5}}$$

is dimensionless, and depends on nothing, i.e., must be a constant. This means that

$$r = C\, \rho^{-1/5} E^{1/5} t^{2/5},$$

or

$$\log r = \log C - \frac{1}{5}\log \rho + \frac{1}{5}\log E + \frac{2}{5}\log t.$$

Thus, if we plot $\log r$ versus $\log t$, the slope should be $2/5$, and the graph should intersect zero at the value

$$\log C - \frac{1}{5}\log \rho + \frac{1}{5}\log E.$$

Since ρ is known, knowing the constant C would reveal the energy of the blast.

In the 1940's the Americans performed nuclear tests, which were photographed by J. Mack. Those photographs were not classified. G.I. Taylor analyzed those pictures. He knew that the constant C was about $O(1)$ (one can find it from a small explosion), and based on the above analysis published the value of the energy (about 10^{21} ergs) which caused a huge embarrassment. ▲

Chapter 2

Newtonian Mechanics

In this chapter we will review the basics of Newton's "old" classical mechanics—old in the sense that it is less general and formal than the more recent formulations of Lagrange and Hamilton—classical, to distinguish from quantum mechanics.

2.1 Kinematics

Mechanics primarily deals with the motion of so-called ***point particles***. A point particle is a ***model*** of a physical object whose state is fully specified by its ***location***, the latter being a point in $\mathbb{R}^3$. It is important to distinguish between models and reality. The point particle is an idealization, which can only be justified empirically. At times, the solar system can be described as comprised of point particles, even though the sun and the planets are complex objects. In other instances, even a round tennis ball cannot be modeled as a point particle (e.g., if rotation is important).

Physics make predictions about how physical entities evolve in time. Given a point particle, its evolution is completely determined by its position $\mathbf{r} = (x, y, z)$, as function of time t, or its ***trajectory***. Mathematically, the trajectory $\mathbf{r}(t)$ is a ***path*** in $\mathbb{R}^3$. For the time being, we will assume that the trajectory is at least twice differentiable with respect to time; the justification for this assumption will be given in the next section.

Note that the definition of $\mathbf{r}$ assumes the choice of an origin, with a specific orientation of the principal axes. In order to be able to measure $\mathbf{r}$ we also need a unit

of length. Centimeters and meters are the most common choices (for those who have never heard of inches and feet...). Time also requires an origin and a unit of measurement, seconds being the most standard choice.

The rate-of-change of the position $\mathbf{r}(t)$, is the vector

$$\mathbf{v}(t) = \frac{d\mathbf{r}}{dt}(t),$$

which is called the ***velocity vector*** of the point particle. Note that this is a vector identity, namely,$\mathbf{v} = (v_1, v_2, v_3)$, with

$$v_1 = \frac{dx}{dt}, \qquad v_2 = \frac{dy}{dt}, \qquad \text{and} \qquad v_3 = \frac{dz}{dt}.$$

The measurement of velocity is somewhat "conceptual". We imagine two measurements of position at time t and time $t + \Delta t$, and an approximation to velocity in terms of the change in $\mathbf{r}$ divided by Δt. The actual velocity is the limit where Δt is infinitely small. Despite the fact that the exact velocity can never be measured, this conceptual measurement suffices to assign velocity dimensions of L/T, where L is the dimension of length and T the dimension of time. If we measure length in units of meters and time in units of seconds, then the ratio of $\Delta\mathbf{r}/\Delta t$ is assigned a unit of meters/seconds. This unit has to be understood in the following way: the velocity was determined by a ratio of displacement and time interval, in an experiments in which length was measured in meters and time in seconds.

Note that if we know the velocity as function of time, $\mathbf{v}(t)$, then the position can be retrieved by integration, but only up to a constant translation,

$$\mathbf{r}(t) = \mathbf{r}(t_0) + \int_{t_0}^{t} \mathbf{v}(s)\, ds.$$

If the velocity is constant, $\mathbf{v}(t) = \mathbf{v}$, then the displacement is a linear function of time,

$$\mathbf{r}(t) = \mathbf{r}(t_0) + \mathbf{v}(t - t_0).$$

The time derivative of the velocity, which is the second derivative of the trajectory, is called the ***acceleration*** of the point particle, and is denoted by

$$\mathbf{a}(t) = \frac{d\mathbf{v}}{dt}(t) = \frac{d^2\mathbf{r}}{dt^2}(t).$$

Acceleration has dimensions of L/T^2, and is usually measured in units of $\mathrm{m/sec}^2$ (again, we don't really mean that a meter is divided by the square of a second). Given the acceleration, $\mathbf{a}(t)$, the velocity is given by

$$\mathbf{v}(t) = \mathbf{v}(t_0) + \int_{t_0}^{t} \mathbf{a}(s)\, ds,$$

and the position is given by

$$\mathbf{r}(t) = \mathbf{r}(t_0) + \mathbf{v}(t_0)(t - t_0) + \int_{t_0}^{t} \int_{t_0}^{s} a(\tau)\, d\tau\, ds.$$

When the acceleration is constant $\mathbf{a}(t) = a$, then

$$\mathbf{v}(t) = \mathbf{v}(t_0) + \mathbf{a}(t - t_0),$$

from which we obtain the trajectory,

$$\mathbf{r}(t) = \mathbf{r}(t_0) + \mathbf{v}(t_0)(t - t_0) + \frac{1}{2}\mathbf{a}(t - t_0)^2,$$

which requires the knowledge of the initial position and velocity of the point particle.

Example: It is an empirical fact that bodies experiencing only the forces of gravity have a constant acceleration,

$$\mathbf{a} = (0, 0, -9.81)\, \frac{\mathrm{m}}{\mathrm{sec}^2}$$

regardless of their mass. Here it is assumed that the z-axis points upward, whereas the x, y plane is tangent to the surface of earth. Suppose we are in a flying balloon, and we throw a massive body from the point $(0, 0, 100)\,\mathrm{m}$ with initial velocity $(3, 0, 10)\,\mathrm{m/sec}$. When and where will the body hit the ground?

By the above formula, setting $t_0 = 0$,

$$\mathbf{r}(t) = (0, 0, 100) + (3, 0, 10)t - \frac{1}{2}(0, 0, 9.81)t^2.$$

Componentwise, we have

$$x(t) = 3t, \qquad y(t) = 0, \qquad \text{and} \qquad z(t) = 100 + 10t - \frac{9.81}{2}t^2.$$

"When" is answered by solving the quadratic equation $z(t) = 0$ (the result is measured in seconds). "Where" is answered by $\mathbf{r}(t)$ at the time of impact (the result is measured in meters). Note also that the curve that the trajectory makes is a parabola,

$$z = 100 + 10\,\frac{x}{3} - \frac{9.81}{2}\left(\frac{x}{3}\right)^2.$$

▲

Circular motion Consider a circular trajectory at constant speed,

$$\mathbf{r}(t) = (R\,\cos\omega t, R\,\sin\omega t, 0), \qquad R, \omega > 0.$$

The velocity is given by

$$\mathbf{v}(t) = (-R\omega\,\sin\omega t, R\omega\,\cos\omega t, 0),$$

i.e., $|\mathbf{v}(t)| = R\omega$, whereas the acceleration is

$$\mathbf{a}(t) = (-R\omega^2\,\cos\omega t, -R\omega^2\,\sin\omega t, 0) = -\omega^2\mathbf{r}(t),$$

i.e., $|\mathbf{a}(t)| = R^2\omega$. We took a very particular circular motion, in which the speed $|\mathbf{v}|$ is constant. The acceleration vector is directed toward the center of the circle, and in particular is perpendicular to the velocity vector.

This is more general: for any motion where $|\mathbf{v}(t)|$ is constant,

$$0 = \frac{d|\mathbf{v}|^2}{dt} = 2\mathbf{v}\cdot\frac{d\mathbf{v}}{dt},$$

i.e., $\mathbf{v} \perp \mathbf{a}$.

2.2 Dynamics: Newton's laws

So far, we have only seen definitions, not physical laws. Physical laws are not inferred from a set of axioms, but are rather based on empirical observations. Their value is in the ability to capture a whole set of physical phenomena in a relatively small set of laws.

Recall that a physical law is an equation that relates between physical quantities, each of which can be measured independently. A physical body, for example, has

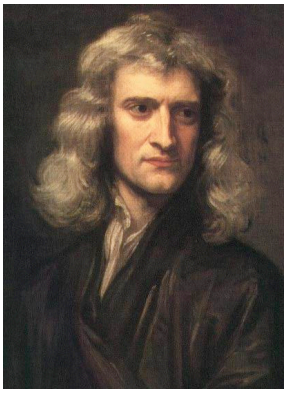


Figure 2.1: Sir Isaac Newton (1643–1727).

a physical quantity associated with—a ***mass***—or the "amount of matter". Mass is commonly measured in units of grams or kilograms (unless you buy it by the ounce), and is denoted by m. The dimension of mass is independent of that of length and time, and we denote it by M.

The product of a particle's mass and velocity, which was once called "the amount of motion" is called the ***momentum*** of the particle, and is denoted by

$$\mathbf{p} = m\mathbf{v}.$$

Momentum is a vector that has dimensions of ML/T.

Newton, in his work *Philosophiae Naturalis Principia Mathematica* (1687), formulated what is now known as Newton's first and second laws of motion: there exist ***frames of references*** in which particles have fixed momenta, unless there is ***force*** exerted on them. When observed from such a reference frame, the rate of change of a particle's momentum is proportional to the (vector) sum of all the forces acting on it. If the total force is denoted by $\mathbf{f}$, then the first and second laws state that

$$\mathbf{f} \propto \frac{d\mathbf{p}}{dt}.$$

Choosing the constant of proportionality amounts to choosing units of measurements. The unit of force Newton is defined as the amount of force needed to change the momentum of a particle at a rate of one kg m/sec per second, in which case we have an equality. Clearly, force has dimensions of ML/T^2. If the mass of

the particle does not change in time, then this law reduces to the celebrated

$$\mathbf{f} = m\mathbf{a}.$$

Note that force, as the derivative of a vector quantity is itself a vector.

But what *is* force? Even Newton realized that he could only give a circular definition. Force is the thing that causes momentum to change, and momentum changes as a result of acting forces. (On the other hand, we certainly have from daily life an intuitive notion of what force is.) Equipped with Newton's second law, the modelling of a mechanical system consists of specifying what the forces are.

Example: For a point particle of mass m kg under only the influence of earth gravity, the force (in Newtons) is

$$\mathbf{f} = -9.81m\,\mathbf{e}_3 \equiv -mg\,\mathbf{e}_3.$$

In this case, Newton's second law reduces to

$$m\mathbf{a} = -mg\mathbf{e}_3,$$

i.e., $\mathbf{a} = -g\,\mathbf{e}_3$, i.e., a constant acceleration independent of the mass. ▲

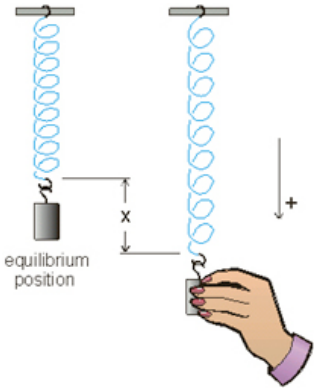
Example: Consider a mass m motionless on a table. Since the body does not accelerate, we must conclude that the total force acting on it zero. Since earth's gravity exerts a constant force $-mg\mathbf{e}_3$ on it, there has to be another force countering it. It is the contact with the table that exerts this countering force, $+mg\,\mathbf{e}_3$. ▲

In many cases, the force on a point particle is a function of its position, $\mathbf{f} = \mathbf{f}(\mathbf{r})$, where $\mathbf{f} : \mathbb{R}^3 \to \mathbb{R}^3$ is a ***vector field***. In this case, Newton's second law is an equation of the form,

$$m\frac{d^2\mathbf{r}}{dt^2} = \mathbf{f}(\mathbf{r}),$$

i.e., a ***second-order ordinary differential system***. Provided that $\mathbf{f}$ is sufficiently regular, this equation has a unique twice-differentiable solution given the initial data $\mathbf{r}(t_0)$ and $\mathbf{v}(t_0)$.

Example:



Consider an ***harmonic oscillator***: a mass m suspended by a spring. The spring has a rest length ℓ; we fix the origin at a vertical distance ℓ from the top of the spring. Assuming that we only consider vertical motion, the total force acting on the mass is

$$\mathbf{f} = (-mg - kz)\mathbf{e}_3,$$

where z is the vertical distance from the origin, and k is a constant associated with the spring. Thus, the trajectory of the mass satisfies the second order differential equation,

$$m\frac{d^2z}{dt^2} = -mg - kz,$$

with initial data $z(0) = z_0$ and $dz/dt(0) = v_0$. This is an inhomogeneous linear equation with constant coefficients. To simplify the solution it is worth to change variables. We first rewrite the equation as

$$\frac{d^2z}{dt^2} = -\frac{k}{m}\left(z + \frac{mg}{k}\right).$$

We then set $w = z + mg/k$, which satisfies the homogeneous differential equation,

$$\frac{d^2w}{dt^2} = -\frac{k}{m}w,$$

with initial data $w(0) = z_0 + mg/k$, and $dw/dt(0) = v_0$. The solution is

$$w(t) = w(0)\,\cos\omega t + \frac{v_0}{\omega}\,\sin\omega t,$$

where $\omega^2 = k/m$. That is, a mass suspended by a spring will perform a periodic sinusoidal motion about the point $z = -mg/k$. ▲

Example: Finally, as an example which we are not going to solve now, we consider the motion of a planet around a massive star. The mass of the planet is m and the mass of the star is M. For the time being, we assume that the star does not move (which is approximately true if $M \gg m$). Newton's ***law of gravitation*** states that the force acting on the planet is directed toward the center of the star, and is given by the well-known ***inverse-square law***,

$$\mathbf{f}(\mathbf{r}) = -GMm\frac{\mathbf{r}}{|\mathbf{r}|^3},$$

where the origin is at the center of the star. G is the universal constant of gravitation. If masses are measured in kilograms, lengths in meters and forces in Newtons, then

$$G = 6.67. \times 10^{-11}\ \frac{\mathrm{N\,m^2}}{\mathrm{kg^2}}.$$

The resulting differential equation

$$m\frac{d^2\mathbf{r}}{dt^2} = -GMm\frac{\mathbf{r}}{|\mathbf{r}|^3}$$

is solvable by analytical means, but we have good reasons to defer its solution to a later stage. ▲

Comment: How does the inverse-square law reconcile with the constant acceleration on earth's surface? If R is earth's radius (6370 kilometers), and $|\mathbf{r}| - R \ll R$, then we can expand the force in Taylor series,

$$\mathbf{f}(\mathbf{r}) = -GMm\frac{\mathbf{r} - R\mathbf{r}/|\mathbf{r}| + R\mathbf{r}/|\mathbf{r}|}{|\mathbf{r}|^3} = -\frac{GMm}{R^2}\left[\left(1 - \frac{R}{|\mathbf{r}|}\right)\frac{\mathbf{r}/R}{|\mathbf{r}/R|^3} + \frac{\mathbf{r}/|\mathbf{r}|}{|\mathbf{r}/R|^3}\right].$$

By assumption, $|\mathbf{r}|/R - 1 \ll 1$, so that up to corrections of that order, the force is well approximated by

$$\mathbf{f}(\mathbf{r}) \approx -\frac{GMm}{R^2}\frac{\mathbf{r}}{|\mathbf{r}|}.$$

Substituting

$$G = 6.67. \times 10^{-11}\ \frac{\mathrm{N\,m^2}}{\mathrm{kg^2}} \qquad M = 5.97\ \times 10^{24}\,\mathrm{kg} \qquad R = 6.37\ \times 10^{6}\,\mathrm{m},$$

we get

$$\mathbf{f}(\mathbf{r}) \approx -\frac{6.67 \times 5.97}{6.37^2} \times 10^{1} m\frac{\mathbf{r}}{|\mathbf{r}|} = -9.81m\frac{\mathbf{r}}{|\mathbf{r}|}.$$

2.3 Work and mechanical energy

Consider a physical body moving under the influence of a force $\mathbf{f}(t)$ (which may be due a force field $\mathbf{f}(\mathbf{r})$. Suppose that the body performs between time t_1 and t_2 a trajectory $\mathbf{r}(t)$. We define the ***work*** exerted on the body as[1]

$$W = \int_{\mathbf{r}} \mathbf{f} \cdot d\mathbf{r} = \int_{t_1}^{t_2} \mathbf{f}(s) \cdot d\mathbf{r}(s) = \int_{t_1}^{t_2} \mathbf{f}(s) \cdot \mathbf{v}(s)\, ds.$$

That is, work is the ***path integral*** of the force along the trajectory. Work may be either positive or negative, where in the latter case we will say that it is the body that has performed work.

In many cases, the force field $\mathbf{f}(\mathbf{r})$ acting on a physical body is ***conservative***. We remind ourselves that a vector field is called conservative if integrals along paths only depend on the end points and not on the trajectory. Moreover, a vector field is conservative if and only if it is the gradient of a scalar field,

$$\mathbf{f} = -\boldsymbol{\nabla}\Phi,$$

where $\Phi(\mathbf{r})$ is called the ***potential field***, or the ***potential energy***; the negative sign is a convention whereby the force is directed in the direction of decreasing potential. For a trajectory $\mathbf{r}$ connecting the points $\mathbf{r}_1$ and $\mathbf{r}_2$,

$$\int_{\mathbf{r}} \mathbf{f} \cdot d\mathbf{r} = -\Phi(\mathbf{r}_2) + \Phi(\mathbf{r}_1).$$

Comment: Recall that the potential is determined only up to an additive constant. Work is independent of this constant.

Example: For a mass under the influence of earth gravity

$$\Phi(\mathbf{r}) = mgz.$$

For a mass suspended on a spring,

$$\Phi(\mathbf{r}) = \frac{1}{2}kz^2.$$

[1]Note the generalization compared with the path integral studied in advanced calculus, the latter always being an integral of a vector field.

For a planet under the influence of a star's gravity,

$$\Phi(\mathbf{r}) = -\frac{GMm}{|\mathbf{r}|}.$$

▲

Consider now a particle of mass m under the influence of a conservative force field. If the particle performs a trajectory $\mathbf{r}(t)$ connecting the points $\mathbf{r}(t_1)$ and $\mathbf{r}(t_2)$ then

$$-\Phi(\mathbf{r}(t_2)) + \Phi(\mathbf{r}(t_1)) = \int_{\mathbf{r}} \mathbf{f} \cdot d\mathbf{r} = m \int_{\mathbf{r}} \mathbf{a} \cdot d\mathbf{r} = m \int_{t_1}^{t_2} \mathbf{a}(s) \cdot \mathbf{v}(s)\, ds,$$

where we have used the definition of the path integral. Noting that

$$\mathbf{a}(t) \cdot \mathbf{v}(t) = \frac{1}{2}\frac{d}{dt}|\mathbf{v}(t)|^2,$$

we obtain

$$-\Phi(\mathbf{r}(t_2)) + \Phi(\mathbf{r}(t_1)) = T(\mathbf{v}(t_2)) - T(\mathbf{v}(t_1)),$$

where

$$T(\mathbf{v}) = \frac{m|\mathbf{v}|^2}{2}$$

is called the ***kinetic energy*** of the particle. Defining the ***total mechanical energy***, or simply the ***energy***,

$$E(\mathbf{r}, \mathbf{v}) = \Phi(\mathbf{r}) + T(\mathbf{v}),$$

we conclude that it assumes the same value at time t_1 and t_2, i.e., it is ***conserved*** (it is a function of the trajectory whose value remains constant in time). Another way to see it is via the chain rule,

$$\frac{d}{dt}E(\mathbf{r}(t), \mathbf{v}(t)) = \frac{d}{dt}\left[\Phi(\mathbf{r}(t)) + \frac{m}{2}|\mathbf{v}(t)|^2\right] = \mathbf{v}(t) \cdot [\boldsymbol{\nabla}\Phi(\mathbf{r}(t)) + m\mathbf{a}(t)] = 0.$$

The conservation of total mechanical energy when forces are conservative is useful as shows the following example:

Example: A body is dropped (at rest) from a height of h meters. At what speed will it hit the ground?

One way to solve it is via the equations of motion: since

$$\frac{d^2z}{dt^2} = -g,$$

with initial data $z(0) = h$ and $dz/dt(0) = 0$, the solution is

$$z(t) = h - \frac{1}{2}gt^2.$$

Thus it hits the ground after time $t_1 = \sqrt{2h/g}$, i.e., $z(t_1) = 0$, and its (vertical) velocity then is

$$v(t_1) = -gt_1 = -\sqrt{2hg}.$$

The other way of solving this exercise is with energies. Taking $\Phi(z) = mgz$, the conservation of energy implies that

$$\Phi(z(0)) + \frac{mv^2(0)}{2} = \Phi(z(t_1)) + \frac{mv^2(t_1)}{2},$$

i.e.,

$$mgh + 0 = 0 + \frac{mv^2(t_1)}{2},$$

which gives the exact same answer. ▲

Example: Earth does not perform any work on the moon because the trajectory of the moon is perpendicular to the vector that connects the moon to the earth, i.e., it is perpendicular to the force of gravity (well, at least approximately). ▲

✎ *Exercise 2.1* Show that for a single particle with constant mass m, Newton's equations imply the following equation for the kinetic energy,

$$\frac{dT}{dt} = \mathbf{f} \cdot \mathbf{v},$$

and more generally, if the mass can vary, then

$$\frac{d(mT)}{dt} = \mathbf{f} \cdot \mathbf{p}.$$

✎ *Exercise 2.2* The escape velocity of a particle on earth is the minimum velocity required in order for a particle to escape from earth's gravitational field. Use the conservation of energy to calculate the escape velocity. Could you obtain this result by directly solving Newton's equations, which for motion along the radial direction take the form,

$$m\frac{d^2r}{dt^2} = -\frac{GMm}{r^2},$$

with initial data $r(0) = R$ and $v(0) = v_0$, where R is the radius of earth?

2.4 Angular momentum and torque

For a particle at position $\mathbf{r}$ having momentum $\mathbf{p}$, we define its ***angular momentum*** as

$$\mathbf{L} = \mathbf{r} \times \mathbf{p}.$$

The importance of this quantity will be seen later on. Note that unlike the momentum, the angular momentum depends on the absolute position of the particle.

The rate of change of the angular momentum can be inferred from Newton's second law, as

$$\frac{d\mathbf{L}}{dt} = \mathbf{v} \times \mathbf{p} + \mathbf{r} \times \frac{d\mathbf{p}}{dt} = \mathbf{r} \times \mathbf{f},$$

where we used the fact that $\mathbf{v} \times \mathbf{p} = m(\mathbf{v} \times \mathbf{v}) = 0$ and Newton's second law. The quantity on the right hand side is called the ***torque*** (or moment of force), and is denoted by

$$\boldsymbol{\tau} = \mathbf{r} \times \mathbf{f}.$$

Thus, the "angular" version of Newton's second law is

$$\frac{d\mathbf{L}}{dt} = \boldsymbol{\tau},$$

i.e., the torque equals to the rate of change of the angular momentum[2].

[2]Up to the dependence of mass, the angular momentum is related to the ***areal velocity***, which is the rate at which area is swept out by the particle.

2.5 Systems of point particles

Until now, we studied a world comprising of a single point mass. We now consider a system comprising of n particles of mass $m_1, \ldots, m_n$. We denote the trajectory of the i-th particle by $\mathbf{r}_i(t)$, its velocity by $\mathbf{v}_i(t)$, and so on[3]. Also, we use $\mathbf{r}$ and $\mathbf{v}$ as short-hand notation for the collections $\{\mathbf{r}_1, \ldots, \mathbf{r}_n\}$ and $\{\mathbf{v}_1, \ldots, \mathbf{v}_n\}$.

Newton's second law states now that every particle satisfies the equation of motion[4],

$$m_i \mathbf{a}_i = \frac{d\mathbf{p}_i}{dt} = \mathbf{f}_i,$$

where $\mathbf{f}_i$ is the total force exerted on the i-th particle. Once again, this does not say much unless the forces $\mathbf{f}_i$ are specified. In many cases, the force acting on the i-th particle can be written as a sum,

$$\mathbf{f}_i = \mathbf{f}_i^e + \sum_{j \neq i} \mathbf{f}_{ji},$$

where $\mathbf{f}_i^e$ stands for an ***external force*** and $\mathbf{f}_{ji}$ is the "internal" force that the j-th particle exerts on the i-th particle. The implicit assumption is that the external force $\mathbf{f}_i^e$ only depends on the position (and perhaps velocity) of the i-th particle, whereas the internal force $\mathbf{f}_{ji}$ only depends on the positions (and perhaps the velocities) of the i-th and j-th particles. Newton's third law, also known as the law of ***action and reaction*** states that the force that the i-th particle exerts on the j-th particle is equal in magnitude but opposite in sign to the force that the j-th particle exerts on the i-th particle

$$\mathbf{f}_{ji} = -\mathbf{f}_{ij}.$$

The distinction between internal and external forces is in a sense arbitrary. It is one's choice which parts of the universe are included in the model, and which are not. External forces represent the interactions between the system and particles that have been left out of our model. An external force could become an internal force by extending the model (e.g., gravity can be viewed as an external force, but also as an internal force if we add earth to our system).

[3] Since we use the notation $\mathbf{r} = (x, y, z)$, we also use $\mathbf{r}_i = (x_i, y_i, z_i)$. On the other hand, we will use $\mathbf{v}_i = (v_{1i}, v_{2i}, v_{3i})$.

[4] Here there is no summation over i. Throughout this section, summations will be denoted explicitly.

Figure 2.2: Pierre Simon Laplace (1749–1827).

Note that once the functions $\mathbf{f}_i^e(\mathbf{r}_i, \mathbf{v}_i)$ and $\mathbf{f}_{ij}(\mathbf{r}_i, \mathbf{r}_j, \mathbf{v}_i, \mathbf{v}_j)$ are specified, we are left with a system of $3n$ second-order ODEs, or, equivalently, a system of $6n$ first-order ODEs. Their solution is uniquely determined by initial data for the positions and velocities of the n particles. It was the French mathematician Pierre-Simon Laplace who pointed out that according to Newton's laws the present uniquely determined both the past and the future: *"We may regard the present state of the universe as the effect of its past and the cause of its future. An intellect which at a certain moment would know all forces that set nature in motion, and all positions of all items of which nature is composed, if this intellect were also vast enough to submit these data to analysis, it would embrace in a single formula the movements of the greatest bodies of the universe and those of the tiniest atom; for such an intellect nothing would be uncertain and the future just like the past would be present before its eyes"*.

Conservation of momentum We turn now to definitions that are pertinent to systems of particles. The ***center of mass*** of a system of particles is a mean position weighted by the mass,

$$\mathbf{R} = \frac{\sum_{i=1}^{n} \mathbf{m_i r_i}}{\sum_{i=1}^{n} \mathbf{m_i}}.$$

The corresponding velocity vector (center-of-mass velocity) is

$$\mathbf{V} = \frac{\mathbf{dR}}{\mathbf{dt}} = \frac{\sum_{i=1}^{n} \mathbf{m_i v_i}}{\sum_{i=1}^{n} \mathbf{m_i}}.$$

If $M = \sum_{i=1}^{n} m_i$ denotes the total mass, then the corresponding momentum,

$$\mathbf{P} = \mathbf{MV} = \sum_{\mathbf{i=1}}^{\mathbf{n}} \mathbf{m_i v_i} = \sum_{\mathbf{i=1}}^{\mathbf{n}} \mathbf{p_i},$$

is simply the (vector) sum of momenta. The rate of change of the total momentum is

$$\frac{d\mathbf{P}}{dt} = \sum_{i=1}^{n} \frac{d\mathbf{p}_i}{dt} = \sum_{i=1}^{n} \left(\mathbf{f}_i^e + \sum_{j \neq i} \mathbf{f}_{ji} \right) = \sum_{i=1}^{n} \mathbf{f}_i^e,$$

where the binary interactions cancel by the law of action and reaction. This amounts to the law of conservation of momentum:

> *In the absence of external force the total momentum of the system is conserved.*

Conservation of angular momentum An analogous conservation law can be derived for the angular momentum. We define the total angular momentum of the system by

$$\sum_{i=1}^{n} \mathbf{r}_i \times \mathbf{p}_i.$$

Now,

$$\frac{d}{dt} \sum_{i=1}^{n} \mathbf{r}_i \times \mathbf{p}_i = \sum_{i=1}^{n} \mathbf{r}_i \times \left(\mathbf{f}_i^e + \sum_{j \neq i} \mathbf{f}_{ji} \right).$$

Consider the terms

$$\sum_{i,j \neq i} \mathbf{r}_i \times \mathbf{f}_{ji}.$$

Since we may interchange the symbols i and j and use the law of action and reaction, this equals

$$\frac{1}{2} \sum_{i,j \neq i} (\mathbf{r}_i - \mathbf{r}_j) \times \mathbf{f}_{ji}.$$

The ***strong law of action and reaction*** states that the force that a particle exerts on another is directed along the line joining the two particles, i.e., $\mathbf{r}_i - \mathbf{r}_j \parallel \mathbf{f}_{ji}$. In such case we have

$$\frac{d}{dt} \sum_{i=1}^{n} \mathbf{r}_i \times \mathbf{p}_i = \sum_{i=1}^{n} \mathbf{r}_i \times \mathbf{f}_i^e.$$

The right-hand side is the total external torque. This leads to the following conservation law,

> *In the absence of external toque the total angular momentum of the system is conserved.*

Conservation of mechanical energy The total work done by all forces is

$$W = \sum_{i=1}^{n} \int_{\mathbf{r}_i} \mathbf{f}_i \cdot d\mathbf{r}_i = \sum_{i=1}^{n} \int_{\mathbf{r}_i} \mathbf{f}_i^e \cdot d\mathbf{r}_i + \sum_{i=1}^{n} \sum_{j \neq i} \int_{\mathbf{r}_i} \mathbf{f}_{ji} \cdot d\mathbf{r}_i.$$

On the other hand,

$$\sum_{i=1}^{n} \int_{\mathbf{r}_i} \mathbf{f}_i \cdot d\mathbf{r}_i = \sum_{i=1}^{n} \int_{t_1}^{t_2} m_i \mathbf{a}_i \cdot \mathbf{v}_i \, dt = T(\mathbf{v}(t_2)) - T(\mathbf{v}(t_1)),$$

where

$$T(\mathbf{v}) = \frac{1}{2} \sum_{i=1}^{n} m_i |\mathbf{v}_i|^2$$

is the ***total kinetic energy***. That is, the total work done by all the forces equals to the gain in total kinetic energy,

$$W = T(\mathbf{v}(t_2)) - T(\mathbf{v}(t_1)).$$

Conservative external forces Consider now the case where the external forces are conservative, i.e.,

$$\mathbf{f}_i^e(\mathbf{r}_i) = -\boldsymbol{\nabla} \Phi_i^e(\mathbf{r}_i),$$

where $\Phi_i^e : \mathbb{R}^3 \to \mathbb{R}$. Then,

$$\sum_{i=1}^{n} \int_{\mathbf{r}_i} \mathbf{f}_i^e \cdot d\mathbf{r}_i = -\sum_{i=1}^{n} \Phi_i^e(\mathbf{r}_i(t_2)) + \sum_{i=1}^{n} \Phi_i^e(\mathbf{r}_i(t_1)).$$

Conservative internal forces Next, consider the case where the internal (binary) forces are conservative. More specifically, we consider the case where the interaction between the i-th and j-th particle is derived from a potential $\Phi_{ij} = \Phi_{ij}(\mathbf{r}_i, \mathbf{r}_j)$, and

$$\mathbf{f}_{ji} = -\boldsymbol{\nabla}_1 \Phi_{ij}(\mathbf{r}_i, \mathbf{r}_j) \qquad \mathbf{f}_{ij} = -\boldsymbol{\nabla}_2 \Phi_{ij}(\mathbf{r}_i, \mathbf{r}_j),$$

where $\boldsymbol{\nabla}_1$ stands for the gradient with respect to the first argument of Φ. By the law of action and reaction $\mathbf{f}_{ij} = -\mathbf{f}_{ji}$, that is,

$$\boldsymbol{\nabla}_1 \Phi_{ij}(\mathbf{r}_i, \mathbf{r}_j) = -\boldsymbol{\nabla}_2 \Phi_{ij}(\mathbf{r}_i, \mathbf{r}_j).$$

What are the implications? What can we say about a function $\phi(x, y)$, satisfying $\partial\phi/\partial x = -\partial\phi/\partial y$? For every x, y we have by the chain rule

$$\frac{d}{ds}\phi(x+s, y+s) = \frac{\partial\phi}{\partial x}(x+s, y+s) + \frac{\partial\phi}{\partial y}(x+s, y+s) = 0,$$

from which we conclude that ϕ is a function of $x - y$[5]. Similarly, in the vector case,

$$\Phi_{ij} = \Phi_{ij}(\mathbf{r}_i - \mathbf{r}_j),$$

that is, the potential only depends on the separation between the two particles.

✎ *Exercise 2.3* Verify that the law of action and reaction (Newton's third law) implies that internal potentials are of the form

$$\Phi_{ij}(\mathbf{r}_i, \mathbf{r}_j) = g(\mathbf{r}_i - \mathbf{r}_j).$$

We also have the *strong* law of action and reaction, which states that

$$\boldsymbol{\nabla}\Phi_{ij}(\mathbf{r}) = g(\mathbf{r})\mathbf{r},$$

where $g : \mathbb{R}^3 \to \mathbb{R}$ is a scalar function. If the gradient of a function is along $\mathbf{r}$, then the function is necessarily constant on spheres centered at the origin, i.e.[6],

$$\Phi_{ij} = \Phi_{ij}(|\mathbf{r}_i - \mathbf{r}_j|).$$

Example: Neutral atoms and molecules exert on each other two main forces: an attractive force at large separations, due to so-called van der Waals forces, and a repulsive force at short separations, due to quantum effects. A simple mathematical model that represents this behavior is the ***Lennard-Jones potential***,

$$\Phi(\mathbf{r}_1, \mathbf{r}_2) = C\left[\left(\frac{\sigma}{|\mathbf{r}_2 - \mathbf{r}_1|}\right)^{12} - \left(\frac{\sigma}{|\mathbf{r}_2 - \mathbf{r}_1|}\right)^{6}\right],$$

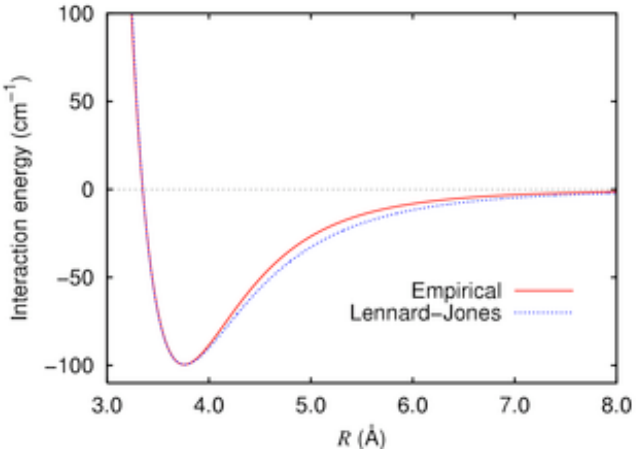


Figure 2.3: The Lennard-Jones potential.

where C, σ are constants pertinent to the specific molecules.

▲

Back to energy conservation. The contribution of the internal forces to the total work is

$$\sum_{i=1}^{n} \sum_{j \neq i} \int_{\mathbf{r}_i} \mathbf{f}_{ji} \cdot d\mathbf{r}_i = -\sum_{i=1}^{n} \sum_{j \neq i} \int_{t_1}^{t_2} \nabla_i \Phi_{ij}(|\mathbf{r}_i(t) - \mathbf{r}_j(t)|) \cdot \mathbf{v}_i(t)\, dt$$
$$= -\sum_{\text{pairs } i,j} \int_{t_1}^{t_2} \nabla_i \Phi_{ij}(|\mathbf{r}_i(t) - \mathbf{r}_j(t)|) \cdot (\mathbf{v}_i(t) - \mathbf{v}_j(t))\, dt.$$

Noting that

$$\nabla_i \Phi_{ij}(|\mathbf{r}_i(t) - \mathbf{r}_j(t)|) \cdot (\mathbf{v}_i(t) - \mathbf{v}_j(t)) = \frac{d}{dt} \Phi_{ij}(|\mathbf{r}_i(t) - \mathbf{r}_j(t)|),$$

we conclude that that total work is given by

$$W = -\Phi(\mathbf{r}(t_2)) + \Phi(\mathbf{r}(t_1)),$$

[5] Set $s = 0$ and $s = -y$ to get that $\phi(x, y) = \phi(x - y, 0) \equiv \psi(x - y)$.

[6] What we have shown is that the function $\Phi_{ij}(\mathbf{r}_i, \mathbf{r}_j)$, which is a function $\mathbb{R}^3 \times \mathbb{R}^3 \to \mathbb{R}$, can be represented as

$$\Phi_{ij}(\mathbf{r}_i, \mathbf{r}_j) = g_{ij}(|\mathbf{r}_i - \mathbf{r}_j|),$$

where $g_{ij} : \mathbb{R} \to \mathbb{R}$. By an abuse of notation we denote this g_{ij} by Φ_{ij} as well.

where $\Phi(\mathbf{r})$ is the ***total potential energy***, given by

$$\Phi(\mathbf{r}) = \sum_{i=1}^{n} \Phi_i^e(\mathbf{r}_i) + \sum_{\text{pairs } i,j} \Phi_{ij}(|\mathbf{r}_i - \mathbf{r}_j|).$$

Since the total work equals to the gain in total kinetic energy, we obtain once more the conservation of total mechanical energy, $E(\mathbf{r}, \mathbf{v}) = \Phi(\mathbf{r}) + T(\mathbf{v})$.

2.6 What is missing?

At this point, one may feel that we have a complete theory of mechanics. A system is a collection of point masses; if we know all the internal and external forces as function of the state of the system, then all we need is initial data, and solve a set of ODEs,

$$m_i \frac{d^2\mathbf{r}_i}{dt^2} = \mathbf{f}_i^e(\mathbf{r}_i) + \sum_{j \neq i} \mathbf{f}_{ji}(\mathbf{r}_i, \mathbf{r}_j).$$

This is indeed the case for, say, stellar mechanics, where $\mathbf{f}_i^e = 0$ and the interaction forces are derivable from a potential,

$$\Phi_{ij}(\mathbf{r}_i, \mathbf{r}_j) = -\frac{Gm_i m_j}{|\mathbf{r}_i - \mathbf{r}_j|},$$

namely,

$$\mathbf{f}_{ji}(\mathbf{r}_i, \mathbf{r}_j) = -\frac{Gm_i m_j}{|\mathbf{r}_i - \mathbf{r}_j|^3}(\mathbf{r}_i - \mathbf{r}_j).$$

✎ *Exercise 2.4* Read about the ***3-body problem*** (search the web; much of that is associated with Poincaré).

Constraints One thing missing in the current picture are ***constraints***. To clarify the issue we consider several examples:

Example: The first example is a body sliding down a slope, as depicted in Figure 2.4. By an appropriate choice of axes, the motion can be restricted to the xz-plane, so that $\mathbf{r} = (x, z)$ will be viewed as two dimensional. If we try to write the equations of motion, we immediately face a problem: earth's gravitation exerts on the body a force $-mg\,\mathbf{e}_2$, but what about the contact with the slope? The

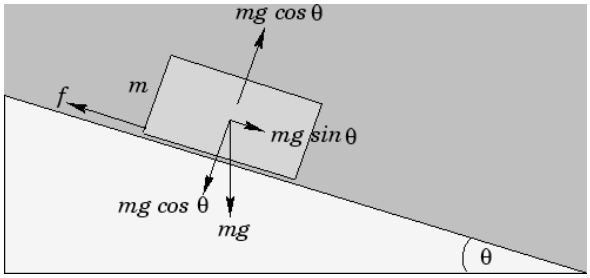


Figure 2.4: A body sliding down a slope.

force of contact is not a-priori given; it acts such to impose the constraint that the body remains above the plane.

We learn how to solve such problems already in high-school. We assume that the contact forces are always normal to the inclined plane. We then rotate the axes by an angle θ, and declare that the forces normal to the plane cancel each other, whereas a force component of $mg\ \sin\theta$ tangent to the plane causes an acceleration of $g\ \sin\theta$ in this direction.

The disturbing points are the ad-hoc treatment and the extra-assumptions that one has to incorporate. ▲

Example: The second example is that of a pendulum, shown in Figure 2.5. A bead is suspended on a rigid (massless) rod whose upper end is fixed; the bead is free to perform circular motion. Here the role of the rod is to impose the constraint that the trajectory remains on a circle. Rather than working with Cartesian coordinates, it makes sense to parametrize the position of the bead by a single angle, say, θ. The question is what equation $\theta(t)$ satisfies. Once again, the force that the rod exerts on the bead is not a-priori known. This is another example of a problem that high-school students can solve, but nevertheless, leaves us with a feeling that mechanics is an incomplete theory.

▲

We now discuss constraints in a general setting. Constraints can be of various type. One of them is where the positions $\mathbf{r} = \{\mathbf{r}_1, \ldots, \mathbf{r}_n\}$ of the various particles satisfy equations of the form

$$h(\mathbf{r}, t) = 0. \tag{2.1}$$

where $h : \mathbb{R}^{3n+1} \to \mathbb{R}^k$. An example of such constraints are ***rigid bodies***, where

Figure 2.5: A pendulum.

the distances between particles are fixed, that is, for all i, j,

$$|\mathbf{r}_i - \mathbf{r}_j| - d_{ij} = 0.$$

Constraints of the type (2.1) are called ***holonomic***. Constraints that are not of that form are called ***non-holonomic***. A simple example of a non-holonomic constraint, is a particle constrained to remain inside the unit sphere, i.e.,

$$|\mathbf{r}| \leq 1.$$

There is no systematic way to deal with non-holonomic constraints (which is to say that the system is not uniquely defined by the known forces and the non-holonomic constraints). In this course, we will only deal with holonomic ones.

As discussed above, constraints induce two sorts of difficulties: (i) the coordinates are no longer independent, hence the equations of motion have to be compatible with the constraints; (ii) the forces that maintain the constraints are a-priori unknown. They are only characterized through their effect, which is to impose the constraints.

"Generalized coordinates" A system of n particles without constraints lives in a $3n$-dimensional Euclidean space. The presence of, say, k holonomic constraints of the form

$$h_i(\mathbf{r}, t) = 0, \qquad i = 1, \ldots, k,$$

where the h_i are sufficiently "nice" functions, restricts the motion into a $(3n-k)$-dimensional ***manifold***, $\mathcal{M}$, which may itself evolve in time (a manifold is a set that locally looks like a Euclidean space). Thus, it is possible, *at least locally*, to reparametrize the constrained space $\mathcal{M}$, at every given time t, by a set of $3n-k$ coordinates, which we denote by

$$\mathbf{q} = (q_1, \ldots, q_{3n-k}) \in U \subset \mathbb{R}^{3n-k},$$

such that there exists a one-to-one mapping $\varphi : U \to \mathcal{M} \subset \mathbb{R}^{3n}$. Mathematicians would call the pair (U, φ) ***local coordinates*** for the manifold $\mathcal{M}$. Physicist call the coordinates $\mathbf{q}$ ***generalized coordinates*** (generalized, to distinguish from the coordinates in the Euclidean space). Thus, the first difficulty of dependent coordinates can be overcome by the use of generalized coordinates.

Comment: From a physicist's point of view the $\mathbf{q}$'s are generalized coordinates in the sense that they need not have dimensions of length.

Example: Consider a system of two point particles at both ends of a rigid rod of length ℓ. The constrained manifold is

$$\mathcal{M} = \left\{(\mathbf{r}_1, \mathbf{r}_2) \in \mathbb{R}^6 : \ |\mathbf{r}_1 - \mathbf{r}_2| = \ell\right\}.$$

This manifold is homeomorphic to $\mathbb{R}^3 \times \mathbb{S}^2$, and we may choose as generalized coordinates the position of the center of mass and the spherical angles of the vector $\mathbf{r}_2 - \mathbf{r}_1$. ▲

The second difficulty however remains: the forces that restrict the motion to $\mathcal{M}$ are unknown. The goal is to obtain a new formulation of mechanics for constained systems that will not require the knowledge of those forces. I.e., that the system will be completely determined by the specification of the "applied" forces, along with a list of constraints. This cannot be done, obviously, without assuming something about the forces of constraints.

Friction Finally, there is another factor missing in our current formulation of mechanics—friction. Friction is treated in high-school physics in an ad-hoc manner as well. Friction is a force that converts mechanical energy into thermal energy, whose nature is outside the scope of mechanics. Thermal energy is a term describing the microscopic motion of the molecules that form a physical body. Conceptually, if we included in our model every single molecule (ignoring the laws of quantum mechanics), there would be no such thing as thermal energy. We will deliberately leave frictional forces outside the scope of the present course.

2.7 d'Alembert's principle of virtual work

First, let us rewrite Newton's second law in a more compact form. If we define a diagonal $3n$-by-$3n$ ***mass matrix***, M, whose diagonal elements are $(m_1, m_1, m_1, m_2, \ldots, m_n)$, then Newton's law can be written in the compact form,

$$M\frac{d^2\mathbf{r}(t)}{dt^2} = \mathbf{f}^{(a)}(\mathbf{r}(t), t) + \mathbf{f}^{(c)}(\mathbf{r}(t), t),$$

where the $3n$-vectors $\mathbf{f}^{(a)}(\mathbf{r}(t), t)$ and $\mathbf{f}^{(c)}(\mathbf{r}(t), t)$ are the forces, which we have split into "applied" forces, and forces of constraints. The applied forces are assumed to be prescribed, whereas the forces of constraints are a-priori unknown.

Suppose then that we have k holonomic constraints, in general time dependent,

$$h_i(\mathbf{r}, t) = 0, \qquad i = 1, \ldots, k,$$

and that the constrained manifold $\mathcal{M}(t)$ is parametrized with $d = 3n-k$ generalized coordinates, $\mathbf{q} = (q_1, \ldots, q_d)$, with the (generally time-dependent) mappings,

$$\mathbf{r} = \boldsymbol{\varphi}(\mathbf{q}, t),$$

where $\boldsymbol{\varphi} : \mathbb{R}^d \times \mathbb{R} \to \mathbb{R}^{3n}$. The assumption that the the constraints define a d-dimensional manifold implies that this relation can be inverted—that $(\mathbf{r}, t)$ defines uniquely $(\mathbf{q}, t)$.

Our goal is to reformulate Newton's equations system as

① A system of equations for the generalized coordinates $\mathbf{q}(t)$.

② In a way that does not require an explicit knowledge of the forces of constraint.

We re-emphasize that this cannot follow from any previous law. One needs to make new assumptions that would tell us how to cope with forces of constraints.

Example: As a simple example, consider a mass suspended on a rod of length ℓ, only allowed to move in the xz-plane, while the upper end of the rod moves upward with velocity u. Thus, $\mathbf{r} = (x, y, z)$ satisfies the constraints,

$$\begin{aligned} h_1(x, y, z, t) &= y = 0 \\ h_2(x, y, z, t) &= x^2 + (z - ut)^2 - \ell^2 = 0. \end{aligned}$$

Figure 2.6: Jean le Rond d'Alembert (1717–1783).

Here we have $n = 1$, $k = 2$ and $d = 3n - k = 1$, At any time t, the particle is constrained to move on a circle (but the circle changes with time), which is a one-dimensional manifold parametrized by an angle θ. The relation between the generalized coordinate θ and the Cartesian coordinate $\mathbf{r}$ is

$$\mathbf{r} = \boldsymbol{\varphi}(\theta, t) = (\ell \sin\theta, 0, ut - \ell \cos\theta).$$

▲

This additional principle was proposed by Jean le Rond d'Alembert, and is known as the principle of ***virtual work***. His principle states the following. At any time t, the velocity vector is constrained to be in a d-dimensional hyper-plane. The forces of constrains, according to d'Alembert's principle, are normal to this hyper-plane. Note that there is only one *actual* velocity vector; the d-dimensional hyper-plane contains all those directions of motion that do not violate the constrains. Such motions are called ***virtual motions***. d'Alembert's principle states that even if the system adopted any of those virtual motions, rather than the actual motion, the forces of constraints would not perform any work. For that reason, d'Alembert's principle is called the principle of virtual work.

D'alembert's principle is a physicist's interpretation of a geometric statement. Given a point $\mathbf{q}$ at time t, any vector

$$\frac{\partial \boldsymbol{\varphi}}{\partial q_j}(\mathbf{q}, t), \qquad j = 1, \ldots, d,$$

is tangent to the constrained manifold. D'alembert's principle states that for every

$j = 1, \ldots, d$,

$$\mathbf{f}^{(c)}(\mathbf{r}(t), t) \perp \frac{\partial \boldsymbol{\varphi}}{\partial q_j}(\mathbf{q}(t), t).$$

Thus, taking the scalar product of Newton's equation with each of those d tangent vectors, we obtain

$$M\frac{d^2\mathbf{r}(t)}{dt^2} \cdot \frac{\partial \boldsymbol{\varphi}}{\partial q_j}(\mathbf{q}(t), t) = \mathbf{f}^{(a)}(\mathbf{r}(t), t) \cdot \frac{\partial \boldsymbol{\varphi}}{\partial q_j}(\mathbf{q}(t), t),$$

where $\mathbf{r}(t)$ and $\mathbf{q}(t)$ are linked by the relation $\mathbf{r}(t) = \boldsymbol{\varphi}(\mathbf{q}(t), t)$.

These are d equations, which we view as equations for the d variables $\mathbf{q}(t)$. We have successfully used d'Alembert's principle to eliminate the forces of constraints. What remains to be done it to express the resulting equations such that only $\mathbf{q}(t)$ appears. In principle, we can do it "brutally" by applying the chain rule, but with some subtlety, we can obtain a nice-looking set of equations.

First, let us rewrite the equations in component form. Also, let us plug in the assumption that all applied forces are derived from a (possibly time-dependent) potential, $\Phi(r, t)$. Then,

$$v_k(t) = \frac{dr_k(t)}{dt}$$
$$m_{ik}\frac{dv_k(t)}{dt}\frac{\partial \varphi_i}{\partial q_j}(\mathbf{q}(t), t) = -\frac{\partial \Phi}{\partial r_i}(\mathbf{r}(t), t)\frac{\partial \varphi_i}{\partial q_j}(\mathbf{q}(t), t).$$

Since

$$r_k(t) = \varphi_k(\mathbf{q}(t), t),$$

it follows that

$$v_k(t) = \frac{\partial \varphi_k}{\partial t}(\mathbf{q}(t), t) + \frac{\partial \varphi_k}{\partial q_\ell}(\mathbf{q}(t), t)\frac{dq_\ell(t)}{dt}.$$

In the same way as we can write the $3n$ second-order equations for $\mathbf{r}(t)$ as $6n$ first order equations for $(\mathbf{r}(t), \mathbf{v}(t))$, we will write the new equations as $2d$ first-order equations for $(\mathbf{q}(t), \dot{\mathbf{q}}(t))$, where we view the variables $\dot{\mathbf{q}}$ as entities independent of $\mathbf{q}$. $3d$ of those equations are then

$$\frac{d\mathbf{q}(t)}{dt} = \dot{\mathbf{q}}(t). \tag{2.2}$$

Then, in the same way as $\mathbf{r}$ and $\mathbf{q}$ are connected by $\boldsymbol{\varphi}$, the pair $(\mathbf{r}, \mathbf{v})$ and $(\mathbf{q}, \dot{\mathbf{q}})$ are connected by

$$r_k = \varphi_k(\mathbf{q}, t) \qquad v_k = \frac{\partial \varphi_k}{\partial t}(\mathbf{q}, t) + \frac{\partial \varphi_k}{\partial q_\ell}(\mathbf{q}, t)\dot{q}_\ell.$$

It will be convenient to redefine now $\mathbf{v}$ as a function of $(\mathbf{q}, \dot{\mathbf{q}}, t)$, as above, in which case we can write the $3d$ equations of motion as

$$m_{ij}\left(\frac{d}{dt}v_k(\mathbf{q}(t), \dot{\mathbf{q}}(t), t)\right)\frac{\partial \varphi_i}{\partial q_j}(\mathbf{q}(t), t) = -\frac{\partial \Phi}{\partial r_i}(\boldsymbol{\varphi}(\mathbf{q}(t), t), t)\frac{\partial \varphi_i}{\partial q_j}(\mathbf{q}(t), t), \tag{2.3}$$

which together with (2.2) forms a closed system of $2d$ equations for $(\mathbf{q}(t), \dot{\mathbf{q}}(t))$.

Let's start with the right-hand side, which can be brought for the more compact form

$$-\frac{\partial \Phi}{\partial q_j}(\boldsymbol{\varphi}(\mathbf{q}(t), t), t).$$

Next, consider the left-hand side, and note first that

$$\frac{\partial v_i}{\partial \dot{q}_j}(\mathbf{q}, \dot{\mathbf{q}}, t) = \frac{\partial \varphi_i}{\partial q_j}(\mathbf{q}, t).$$

The left-hand side takes the form

$$m_{ik}\frac{d}{dt}\left(v_k(\mathbf{q}(t), \dot{\mathbf{q}}(t), t)\frac{\partial v_i}{\partial \dot{q}_j}(\mathbf{q}(t), \dot{\mathbf{q}}(t), t)\right) - m_{ik}v_k(\mathbf{q}(t), \dot{\mathbf{q}}(t), t)\frac{d}{dt}\frac{\partial \varphi_i}{\partial q_j}(\mathbf{q}(t), t).$$

By introducing the function

$$T(\mathbf{q}, \dot{\mathbf{q}}, t) = \frac{1}{2}m_{ik}v_i(\mathbf{q}, \dot{\mathbf{q}}, t)\, v_k(\mathbf{q}, \dot{\mathbf{q}}, t),$$

we can rewrite the first term as

$$\frac{d}{dt}\left[\frac{\partial T}{\partial \dot{q}_j}(\mathbf{q}(t), \dot{\mathbf{q}}(t), t)\right].$$

As for the second term we note that

$$\begin{aligned}\frac{d}{dt}\frac{\partial \varphi_i}{\partial q_j}(\mathbf{q}(t), t) &= \frac{\partial^2 \varphi_i}{\partial q_j \partial q_\ell}(\mathbf{q}(t), t)\dot{q}_\ell(t) + \frac{\partial^2 \varphi_i}{\partial q_j \partial t}(\mathbf{q}(t), t) \\ &= \frac{\partial v_i}{\partial q_j}(\mathbf{q}(t), \dot{\mathbf{q}}(t), t),\end{aligned}$$

so that the second term is

$$-\frac{\partial T}{\partial q_j}(\mathbf{q}(t), \dot{\mathbf{q}}(t), t).$$

At this point, we rewrote the equations of motion as

$$\frac{d}{dt}\left[\frac{\partial T}{\partial \dot{q}_j}(\mathbf{q}(t), \dot{\mathbf{q}}(t), t)\right] - \frac{\partial T}{\partial q_j}(\mathbf{q}(t), \dot{\mathbf{q}}(t), t) = -\frac{\partial \Phi}{\partial q_j}(\boldsymbol{\varphi}(\mathbf{q}(t), t), t).$$

Defining a function of $(\mathbf{q}, \dot{\mathbf{q}}, t)$, which we call the ***Lagrangian***,

$$L(\mathbf{q}, \dot{\mathbf{q}}, t) = T(\mathbf{q}, \dot{\mathbf{q}}, t) - \Phi(\boldsymbol{\varphi}(\mathbf{q}, t), t),$$

The generalized coordinates satisfy the d coupled equations,

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}_k}\right) - \frac{\partial L}{\partial q_k} = 0. \tag{2.4}$$

By the end of tedious calculus manipulations, we have obtained a closed set of equations for only the generalized coordinates; they are known as the ***Euler-Lagrange equations***. Writing these equations explicitly only requires the knowledge of a scalar valued function—the Lagrangian—in terms of the generalized coordinates and the generalized velocities.

2.8 Examples

Example: Our first example is a pendulum: a mass m hung on a rigid rod of length ℓ, whose (upper) end is fixed. The mass is free to move on a circle of radius ℓ on the xz-plane. We only need one generalized coordinate: the angle that the rod makes with the vertical axis. The relation between $\mathbf{r}$ and θ is

$$\mathbf{r} = \boldsymbol{\varphi}(\theta) = (\ell \sin\theta, 0, -\ell \cos\theta),$$

hence

$$\mathbf{v} = (\ell \cos\theta, 0, \ell \sin\theta)\dot{\theta},$$

and the kinetic energy is given by

$$T = \frac{m\ell^2}{2}\dot{\theta}^2.$$

The potential energy is given by

$$\Phi = mgz = -mg\ell\cos\theta,$$

so that the Lagrangian is

$$L(\theta, \dot{\theta}, t) = \frac{m\ell^2}{2}\dot{\theta}^2 + mg\ell\cos\theta.$$

The evolution of $\theta(t)$ is determined by (2.4),

$$\frac{d}{dt}(m\ell^2\dot{\theta}) + mg\ell\sin\theta = 0,$$

or,

$$\ddot{\theta} = -\frac{g}{\ell}\sin\theta.$$

(For small angles it is standard to approximate $\sin\theta \approx \theta$.) ▲

Example: Suppose now that this pendulum is free to move on the sphere defined by the distance ℓ from the anchor point (i.e., a two-dimensional manifold). We parametrize the location of the mass by the two spherical angles (θ, ϕ) with

$$\mathbf{r} = \boldsymbol{\varphi}(\theta, \phi) = \ell\,(\sin\theta\cos\phi, \sin\theta\sin\phi, -\cos\theta),$$

hence

$$\dot{r} = \ell\,(\cos\theta\cos\phi, \cos\theta\sin\phi, \sin\theta)\,\dot{\theta} + \ell\,(-\sin\theta\sin\phi, \sin\theta\cos\phi, 0)\,\dot{\phi},$$

and the kinetic energy is given by

$$T = \frac{m\ell^2}{2}\left(\dot{\theta}^2 + \sin^2\theta\,\dot{\phi}^2\right).$$

The potential energy, on the other hand, is still given by

$$\Phi = mgz = -mg\ell\cos\theta,$$

so that the Lagrangian is

$$L(\theta, \dot{\theta}, \phi, \dot{\phi}, t) = \frac{m\ell^2}{2}\left(\dot{\theta}^2 + \sin^2\theta\,\dot{\phi}^2\right) + mg\ell\cos\theta.$$

The equations of motion are therefore,

$$\frac{d}{dt}(m\ell^2\dot{\theta}) - \frac{m\ell^2}{2}\sin 2\theta\dot{\phi}^2 + mg\ell\sin\theta = 0$$

$$\frac{d}{dt}(m\ell^2\sin^2\theta\,\dot{\phi}) = 0.$$

▲

Figure 2.7: An Atwood machine

Example: Consider now the pendulum where the anchor point is pulled upward with velocity a. Now we have

$$\boldsymbol{\varphi}(\mathbf{q}, t) = (\ell \sin\theta, 0, at - \ell\cos\theta).$$

Note that we end up with the exact same dynamics. ▲

✎ *Exercise 2.5* Consider a mass m suspected by a rod of length ℓ and free to move in the xz plane. The upper end of the rod undergoes "forced" oscillations in the vertical axis; it position is given by

$$z(t) = \cos\omega_0 t,$$

where ω_0 is a constant. The goal is to describe the motion of the suspended mass. (i) Choose generalized coordinates. (ii) Write the Lagrangian. (iii) Write the equations of motion. (iv) Try to solve them.

✎ *Exercise 2.6* Use the Lagrangian formalism to write the equations of motion of two point particles of mass m and M connected by a rigid rod of length ℓ, falling under the influence of gravity.

Example: The ***Atwood machine*** was invented in 1784 by George Atwood as a laboratory experiment to verify the mechanical laws of uniformly accelerated motion.

Consider a simple Atwood machine with a mass m_1 at one end of the string and a mass m_2 at the other end. The state of the system may be parametrized with a single coordinate, say, z, which is the vertical coordinate of the mass m_1 relative to the point where both are at the same height. Here we have

$$\mathbf{r}_1 = \boldsymbol{\varphi}_1(z) = (-a, 0, z)$$
$$\mathbf{r}_2 = \boldsymbol{\varphi}_2(z) = (a, 0, -z),$$

where, without loss of generality, we have assumed that the horizontal separation is $2a$ along the x-axis. The Lagrangian is

$$L(z, \dot{z}, t) = \frac{m_1}{2}\dot{z}^2 + \frac{m_2}{2}\dot{z}^2 + m_1 g z - m_2 g z,$$

and the corresponding equations of motion are

$$(m_1 + m_2)\ddot{z} - (m_1 - m_2)g = 0,$$

namely,

$$\ddot{z} = \frac{m_1 - m_2}{m_1 + m_2} g.$$

Note that the acceleration is relative to the normalized mass difference. ▲

✎ *Exercise 2.7* Consider a bead sliding (without friction) on a rotating wire in a force-free space (i.e., no gravity). Specifically, consider a straight wire rotated at constant angular speed about a fixed axis perpendicular to the wire. (1) Choose generalized coordinates. (2) Establish the relation between the generalized coordinates and the Cartesian coordinates. (3) Write the Lagrangian. (4) Write the corresponding equations of motion. (5) Solve the equations. (6) Provide an "intuitive" interpretation of the result.

Chapter 3

Variational Calculus

3.1 The brachistochrone

The name of this classical problem comes from Greek ($\beta\rho\alpha\chi\iota\sigma\tau\omicron\varsigma$ means shortest and $\chi\rho\omicron\nu\omicron\varsigma$ means time). It is the first variational problem that has even been formulated. It was first solved by Johann Bernoulli, who posed it to readers of Acta Eruditorum in June 1696. Four mathematicians responded with solutions: Isaac Newton, Jakob Bernoulli, Gottfried Leibniz and Guillaume de l'Hôpital.

The problem is the following: Let $P_1 = (0, 0)$ and $P_2 = (1, -1)$ be two points in $\mathbb{R}^2$. We connect these two points by a continuously differentiable curve $y = f(x)$. Suppose that a bead was allowed to slid frictionless along this curve, what is the curve for which the time that it takes to reach the point P_2 is minimal? We assume that the only *applied* force is gravity. See Figure 3.1 for a visualization.

The bead performs a motion $(x(t), y(t))$, where $y(t) = f(x(t))$. The velocity is therefore

$$v_1(t) = \dot{x}(t) \qquad v_2(t) = \dot{y}(t) = f'(x(t))\,\dot{x}(t),$$

i.e.,

$$|\mathbf{v}(t)| = \sqrt{1 + [f'(x(t))]^2}\,\dot{x}(t).$$

Conservation of mechanical energy[1] implies that

$$\frac{1}{2}m|\mathbf{v}(t)|^2 = -mgy(t),$$

[1] At this point, we are not concerned about the laws of physics. The variational problem can be posed irrespectively of its mechanical origin.

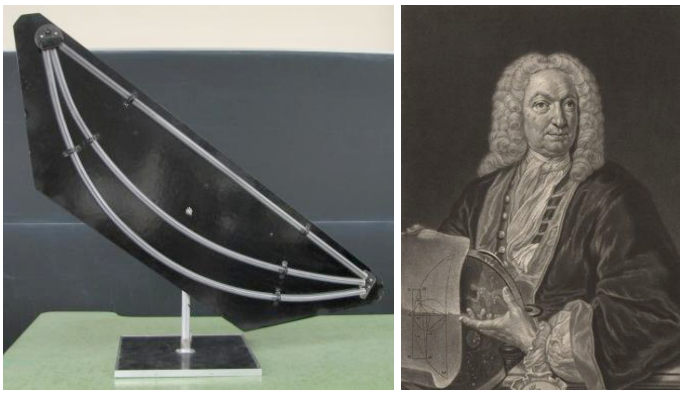


Figure 3.1: An experimental demonstration of the brachistochrone and its inventor, Johann Bernoulli (1667–1748).

so that

$$\sqrt{1 + [f'(x(t))]^2}\, \dot{x}(t) = \sqrt{-2gf(x(t))},$$

or,

$$\frac{\sqrt{1 + [f'(x(t))]^2}}{\sqrt{-2gf(x(t))}}\, \dot{x}(t) = 1.$$

Integrating over time from $t = 0$ to $t = T$, the time it takes to reach the point P_2, we get

$$T = \int_0^1 \frac{\sqrt{1 + [f'(x)]^2}}{\sqrt{-2gf(x)}}\, dx.$$

This is the quantity to be minimized. We are looking for a function $f(x)$ satisfying $f(0) = 0$, $f(1) = -1$, which minimizes this integral. For those who graduated from our calculus course, this is a totally new problem. We are asked to minimize a function of a function, i.e., the space over which we seek the minimum is infinite-dimensional. We will soon have the tools to answer this question.

✎ *Exercise 3.1* Formulate mathematically the problem of finding the shortest curve that connects two points in the plane.

3.2 Functionals over normed spaces

In the preceding section we were required to minimize a real-valued function of a function. Such objects are called ***functionals***.

Definition 3.1 *Let $\mathscr{X}$ be a normed linear space. A functional on $\mathscr{X}$ is a mapping $\mathscr{X} \to \mathbb{R}$, i.e., a real valued function.*

In the course on advanced calculus we deal with functions between arbitrary metric spaces. Recall that any normed space has an induced metric. In particular, we have a well-defined notion of continuity of such mappings.

Definition 3.2 *Let $\mathscr{X}$ be a normed linear space. The set of all continuous linear functionals $\mathscr{X} \to \mathbb{R}$ is called the space* ***dual*** *to $\mathscr{X}$ and is denoted by $\mathscr{X}^*$.*

Example: Let $\mathscr{X} = C^1[0,1]$ be the space of continuously-differentiable functions on $[0,1]$ with the norm

$$\|f\| = \sup_{0\le x\le 1} |f(x)| + \sup_{0\le x\le 1} |f'(x)|.$$

The following is a functional on $\mathscr{X}$,

$$I[f] = \int_0^1 \left[f^2(x) + f(x)f'(x)\right] dx.$$

We can show that it is in fact continuous. Let (f_n) be a sequence of functions that converges to f in $C^1[0,1]$. Then,

$$I[f_n] - I[f] = \int_0^1 (f_n - f)(f_n + f)\, dx + \int_0^1 f_n(f_n' - f')\, dx + \int_0^1 (f_n - f)f'\, dx.$$

Because the sequence f_n is convergent, it is bounded (call the common bound of f_n and f, C), and we can bound this difference by

$$|I[f_n] - I[f]| \le 4C\|f_n - f\| \to 0.$$

▲

✎ *Exercise 3.2* Show that

$$\|f\| = \sup_{0\le x\le 1} |f(x)| + \sup_{0\le x\le 1} |f'(x)|$$

is a norm on $C^1[0,1]$.

Example: Let again $\mathscr{X} = C[0,1]$. The following functional is called the δ-***measure*** concentrated at $x = 1/2$,

$$I[f] = f(\tfrac{1}{2}).$$

It is clearly a linear functional, and it is continuous on $\mathscr{X}$. Physicists call it the ***Dirac delta-function*** and denote it by

$$I[f] = \int_0^1 \delta(x - \tfrac{1}{2}) f(x)\, dx.$$

It should be emphasized that there is no such function δ, and that this is a mere notation. ▲

3.3 Functional derivatives

In the advanced calculus course we only developed differential calculus for functions between finite-dimensional normed spaces. We will now generalize the concept of differentiability for functionals over infinite-dimensional normed spaces.

Definition 3.3 Let $\mathscr{X}$ be a normed space. A functional $I : \mathscr{X} \to \mathbb{R}$ is said to be ***Fréchet differentiable*** *at f if there exists a continuous linear functional $T : \mathscr{X} \to \mathbb{R}$, such that*

$$\lim_{g \to 0} \frac{I[f+g] - I[f] - T[g]}{\|g\|} = 0.$$

Naturally, we can denote $T = D_I(f)$.

Example: Let $\mathscr{X} = C[0,1]$ and consider the functional

$$I[f] = \int_0^1 f^2(x)\, dx.$$

We claim that I is Fréchet differentiable with

$$D_I(f)[g] = \int_0^1 f(x)g(x)\, dx.$$

To show that we first need to show that $D_I(f)$ is a continuous functional (it is clearly linear), that it, that if $g_n \to g$ in $C[0,1]$, then $D_I(f)[g_n] \to D_I(f)[g]$ in $\mathbb{R}$. Indeed,

$$|D_I(f)[g_n] - D_I(f)[g]| = \left| \int_0^1 f(x)[g_n(x) - g(x)]\,dx \right| \leq \|f\|\,\|g_n - g\| \to 0.$$

Finally, we need to show that

$$\lim_{g\to 0} \frac{I[f+g] - I[f] - D_I(f)[g]}{\|g\|} = 0,$$

and indeed,

$$\frac{I[f+g] - I[f] - D_I(f)[g]}{\|g\|} = \frac{\int_0^1 g^2(x)\,dx}{\|g\|} \leq \|g\| \to 0.$$

▲

✎ *Exercise 3.3* Prove that

$$I[f] = \int_0^1 f^n(x)\,dx,$$

is Fréchet differentiable on $C[0,1]$. What is the derivative?

Recall that for functions between finite-dimensional normed spaces differentiability implies the existence of ***directional derivatives***, but the converse is not necessarily true. Thus, one can define a weaker notion of differentiability, known as ***Gâteaux differentiability***.

Specifically, if I is differentiable at $f \in \mathscr{X}$, then for every $g \in \mathscr{X}$,

$$\lim_{t\to 0} \frac{I[f+tg] - I[f] - t\,D_I(f)[g]}{t} = 0,$$

i.e.,

$$D_I(f)[g] = \lim_{t\to 0} \frac{I[f+tg] - I[f]}{t}.$$

Definition 3.4 Let $\mathscr{X}$ be a normed space. A functional $I : \mathscr{X} \to \mathbb{R}$ is said to be ***Gâteaux differentiable*** *at f if there exists a continuous linear functional $T : \mathscr{X} \to \mathbb{R}$, such that*

$$T[g] = \lim_{t\to 0} \frac{I[f+tg] - I[f]}{t}$$

for all $g \in \mathscr{X}$. We will denote this functional by $\delta I(f)$ (to distinguish from $D_I(f)$).

Example: Let $\mathscr{X} = C^1[0,1]$ and

$$I[y] = \int_0^1 f(x, y(x), y'(x))\, dx,$$

where $f \in C^1(\mathbb{R}^3)$. We will show that I is Gâteaux differentiable at $y \in \mathscr{X}$. For every $z \in \mathscr{X}$,

$$\frac{I[y+tz] - I[y]}{t} = \frac{1}{t} \int_0^1 [f(x, y(x) + tz(x), y'(x) + tz'(x)) - f(x, y(x), y'(x))]\, dx.$$

For every x inside the integral we can use the mean-value theorem,

$$\frac{I[y+tz] - I[y]}{t} = \int_0^1 \left[\frac{\partial f}{\partial y}(\dots) z(x) + \frac{\partial f}{\partial y'}(\dots) z'(x) \right] dx,$$

and as we take $t \to 0$,

$$\delta I(y)[z] = \int_0^1 \left[\frac{\partial f}{\partial y}(x, y(x), y'(x))\, z(x) + \frac{\partial f}{\partial y'}(x, y(x), y'(x))\, z'(x) \right] dx,$$

which is a continuous linear functional on $\mathscr{X}$. ▲

3.4 Necessary conditions for a local extremum

A typical variational problem is the following. Find $y \in \mathscr{X}$ that minimizes

$$I[y] = \int_a^b f(x, y(x))\, dx,$$

such that $y(a) = y_a$ and $y(b) = y_b$. That is, we are only looking for a minimizer among functions

$$\mathscr{K} = \{y \in \mathscr{X} : \ y(a) = y_a, y(b) = y_b\}.$$

It should be noted that the subset $\mathscr{K} \subset \mathscr{X}$ is not even a vector space (unless $y_a = y_b = 0$). Such a set will be called the set of ***competing functions***.

If however we set

$$\mathscr{K}_0 = \{y \in \mathscr{X} : \ y(a) = 0, y(b) = 0\},$$

then it is clear that $\mathscr{K} + \mathscr{K}_0 = \mathscr{K}$ (this is an addition between sets). Functions in $\mathscr{K}_0$ can be view as variations of functions in $\mathscr{K}$ that leave the sum in $\mathscr{K}$. This set will be called the set of ***admissible variations*** of $\mathscr{K}$.

More generally,

Definition 3.5 *Let $\mathscr{K} \subset \mathscr{X}$. The set of admissible variations of $\mathscr{K}$ is defined by*

$$\mathscr{K}_0 = \{z \in \mathscr{X} : \ y + z \in \mathscr{K} \ \forall y \in \mathscr{K}\}.$$

In the above example, the space $\mathscr{K}_0$ of admissible variations is a vector space. This is not always the case.

We will now formulate what exactly is meant by a local minimum (or maximum):

Definition 3.6 *Let $\mathscr{K} \subset \mathscr{X}$ be a space of competing functions, and let I be a functional on $\mathscr{X}$. The function $y \in \mathscr{K}$ is said to be a **local minimum** of I in $\mathscr{K}$, if there exists an open ball $B_0(y, \delta)$, such that*

$$I[y] \leq I[z] \qquad \text{for all } z \in \mathscr{K} \cap B_0(y, \delta).$$

Proposition 3.1 *Let $\mathscr{K} \subset \mathscr{X}$ be a set of competing functions. The function $y \in \mathscr{K}$ is a local minimum of $I : \mathscr{X} \to \mathbb{R}$ in $\mathscr{K}$ **only if** there exists an open ball $B_0(0, \delta)$, such that*

$$I[y] \leq I[y + h] \qquad \text{for all } h \in \mathscr{K}_0 \cap B_0(0, \delta).$$

Proof: The proof is obvious as any such $y + h$ is a z in the definition of the local minimum. ■

Consider now the particular case where I is Gâteaux differentiable and where the space of admissible variations is a linear space. If $y \in \mathscr{K}$ is a local minimum of I in $\mathscr{K}$, then for every admissible variation $h \in \mathscr{K}_0$ there exists a $\delta > 0$ such that

$$I[y + th] \geq I[y] \qquad \text{for all } |t| < \delta.$$

Equivalently,

$$\frac{I[y + th] - I[y]}{t} \geq 0 \qquad \text{for all } 0 < t < \delta$$

$$\frac{I[y + th] - I[y]}{t} \leq 0 \qquad \text{for all } -\delta < t < 0.$$

Since, by assumption, I is Gâteaux differentiable, we conclude that a ***necessary condition*** for y to be a local minimum of I in $\mathscr{K}$ is that

$$\delta I(y)[h] = 0 \qquad \text{for all } h \in \mathscr{K}_0.$$

Another, equivalent, argument is to consider the real-valued function $I[f + th]$. Since it must attain a minimum at $t = 0$ for every $h \in \mathscr{K}_0$, we have

$$\frac{d}{dt} I[f + th]\Big|_{t=0} = 0,$$

which, for a Gâteaux-differentiable functional I amounts to $\delta I(f)[h] = 0$.

We have thus shown the following:

Theorem 3.1 If $I : \mathscr{X} \to \mathbb{R}$ is Gâteaux differentiable, $\mathscr{K} \subset \mathscr{X}$ is a set of competing functions that assumes a vector space $\mathscr{K}_0$ of admissible variations, and $y \in \mathscr{K}$ is a local minimum of I in $\mathscr{K}$, then necessarily,

$$\delta I(y)[h] = 0 \qquad \textit{for all } h \in \mathscr{K}_0.$$

Having defined the first Gâteaux derivative, we can naturally define the second Gâteaux derivative (if it exists) to be the derivative of the first derivative, which is a bilinear functional,

$$\delta^2 I(f)[g, h] = \lim_{t \to 0} \frac{\delta I(f + th)[g] - \delta I(f)[g]}{t}.$$

Now, for $I[f + th]$ to attain a local minimum at $t = 0$, a second necessary condition is

$$\frac{d^2}{dt^2} I[f + th]\Big|_{t=0} > 0,$$

which implies that $\delta^2 I(f)$ is positive-definite,

$$\delta^2 I(f)[h, h] > 0 \qquad \text{for every } h \in \mathscr{K}_0.$$

3.5 The Euler-Lagrange equations

This brings us to our ultimate goal, which is to derive the necessary conditions that a function $y(x)$ has to fulfill in order to minimize a functional

$$I[y] = \int_a^b f(x, y(x), y'(x))\, dx,$$

among all competing functions,

$$\mathscr{K} = \left\{ y \in C^1[a,b] : \ y(a) = y_a, \ y(b) = y_b \right\}.$$

The space of admissible variations is the normed space

$$\mathscr{K}_0 = \left\{ y \in C^1[a,b] : \ y(a) = y(b) = 0 \right\}.$$

We have already seen that

$$\delta I(y)[z] = \int_a^b \left[\frac{\partial f}{\partial y}(x, y(x), y'(x))\, z(x) + \frac{\partial f}{\partial y'}(x, y(x), y'(x))\, z'(x) \right] dx.$$

Take now the second term, and integrate by parts (assuming it is allowed),

$$\begin{aligned} \int_a^b \frac{\partial f}{\partial y'}(x, y(x), y'(x))\, z'(x)\, dx = & \left. \frac{\partial f}{\partial y'}(x, y(x), y'(x))\, z(x) \right|_a^b \\ & - \int_a^b \frac{d}{dx} \left(\frac{\partial f}{\partial y'}(x, y(x), y'(x)) \right) z(x)\, dx. \end{aligned}$$

The boundary terms vanish because $z(x)$ vanishes at the end points. Hence, we remain with

$$\delta I(y)[z] = \int_a^b \left[\frac{\partial f}{\partial y}(x, y(x), y'(x)) - \frac{d}{dx} \left(\frac{\partial f}{\partial y'}(x, y(x), y'(x)) \right) \right] z(x)\, dx.$$

Since this variation has to vanish for all $z \in \mathscr{K}_0$, we conclude that the minimizer $y(x)$ has to satisfy the ***Euler-Lagrange*** equations,

$$\frac{\partial f}{\partial y}(x, y(x), y'(x)) - \frac{d}{dx} \left(\frac{\partial f}{\partial y'}(x, y(x), y'(x)) \right) = 0.$$

This is a second-order ordinary differential equation, which at once reminds us the equations obtained in the previous chapter for the evolution of the generalized coordinates. The connection between these two topics will be made in the next chapter.

✎ *Exercise 3.4* Prove that the line is indeed the shortest path between two points in the plane.

✎ *Exercise 3.5* Solve the brachistochrone problem.

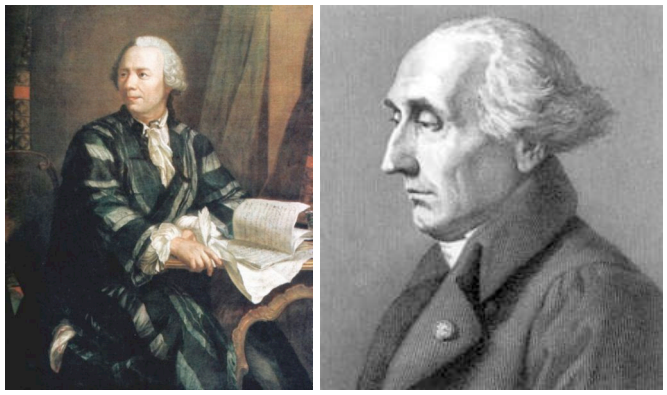


Figure 3.2: Leonhard Euler (1707–1783) and Joseph Louis Lagrange (1736–1813).

Chapter 4

Lagrangian mechanics

4.1 Hamilton's principle

Our ultimate goal is to determine the path $\mathbf{q}(t)$ in the space $\mathbb{R}^d$ of generalized coordinates (the ***configuration space***) that a mechanical systems adopts under the influence of applied forces and (holonomic) constraints. Note that every point $\mathbf{q}(t)$ along this path represents the entire system, and not just, say, a single particle. In Chapter 2, based on d'Alembert's principle of zero virtual work, we derived the Lagrange equations,

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{q}_j} - \frac{\partial L}{\partial q_j} = 0, \qquad j = 1, \ldots, d,$$

where $L(\mathbf{q}, \dot{\mathbf{q}}, t)$ is the Lagrangian of the system, i.e., the kinetic energy minus the potential energy. The Lagrange equations form a second-order differential system in $\mathbb{R}^d$, which needs to be supplemented with suitable initial data.

In this section we obtain the same Lagrange equations from a different governing rule, known as ***Hamilton's principle of least action***. We consider a priori all paths $\mathbf{q}(t)$ between given initial and end points,

$$\mathbf{q}(t_1) = \mathbf{q}_1 \qquad \text{and} \qquad \mathbf{q}(t_2) = \mathbf{q}_2.$$

For each such path, we define a functional, the ***action***,

$$I[\mathbf{q}] = \int_{t_1}^{t_2} L(\mathbf{q}(t), \dot{\mathbf{q}}(t), t)\, dt.$$

Hamilton's principle states that among all those paths, the one that will be selected is the one that minimizes the action. As we've seen, this implies the Lagrange equations.

Comments:

① Hamilton's principle assumes that the end points of the trajectory are known. This yields that the trajectory satisfies a second order system, which can then be supplemented by initial data, yielding a unique solution.

② While the idea that the system is "free to choose" many paths and eventually adopts a selected one, may first sound fictitious. It is remarkable that both in optics and quantum mechanics, waves actually adopt all possible paths, but interference effects cause (in certain limits) the selection of a unique limiting path.

③ Integral principle often have the advantage to remain correct even in situations where their differential counterparts fail (e.g. lack of regularity). As such, they are "more general".

④ Where did we use the fact that the constraints were holonomic? In the assumption that the q_j are algebraically independent. Hamilton's principle can apply also to certain non-holonomic constraints, but we will not get into it.

4.2 Conservation theorems

Recall the conservation of momenta and energy in Newtonian mechanics. One may wonder under what conditions there exist such conserved quantities. In this section we will show that conservation laws reflect symmetries pertinent to the system.

Definition 4.1 *Let $L(\mathbf{q}, \dot{\mathbf{q}}, t)$ be the Lagrangian of a mechanical system. We define*

$$p_j(\mathbf{q}, \dot{\mathbf{q}}, t) = \frac{\partial L}{\partial \dot{q}_j}(\mathbf{q}, \dot{\mathbf{q}}, t)$$

to be the ***generalized momentum*** *conjugate to the generalized coordinate q_j. Moreover, if L does not depend on q_j, the latter is called a* ***cyclic coordinate****.*

Proposition 4.1 *The generalized momentum conjugate to a cyclic coordinate is conserved.*

Proof: Immediate. ■

For example, one can show that the conservation of total momentum follows when the Lagrangian is invariant under a translation of the entire system, whereas the conservation of total angular momentum follows when the Lagrangian is invariant under a rotation of the entire system. ***Noether's theorem*** states that any differentiable symmetry of the action of a physical system has a corresponding conservation law.

Remains the conservation of energy. We start by noting that

$$\frac{d}{dt}L(\mathbf{q}(t),\dot{\mathbf{q}}(t),t)=\sum_{j=1}^{d}\left(\frac{\partial L}{\partial q_j}\dot{q}_j+\frac{\partial L}{\partial \dot{q}_j}\ddot{q}_j\right)+\frac{\partial L}{\partial t}.$$

Substituting the Lagrange equations,

$$\frac{d}{dt}L(\mathbf{q}(t),\dot{\mathbf{q}}(t),t)=\sum_{j=1}^{d}\left(\frac{d}{dt}\frac{\partial L}{\partial \dot{q}_j}\dot{q}_j+\frac{\partial L}{\partial \dot{q}_j}\ddot{q}_j\right)+\frac{\partial L}{\partial t},$$

which we can then turn into

$$\frac{d}{dt}\left(\sum_{j=1}^{d}\dot{q}_j\frac{\partial L}{\partial \dot{q}_j}-L\right)+\frac{\partial L}{\partial t}=0.$$

We then define

$$h(\mathbf{q},\dot{\mathbf{q}},t)=\sum_{j=1}^{d}\dot{q}_j\frac{\partial L}{\partial \dot{q}_j}-L.$$

Proposition 4.2 *If the Lagrangian does not depend on time (i.e., is invariant under an arbitrary translation of time), then the function h is conserved,*

The function h, which will later on play a fundamental role in Hamiltonian mechanics, may be, under certain circumstances, the total energy, $T+\Phi$. Recall that

$$T(\mathbf{q},\dot{\mathbf{q}},t)=\frac{1}{2}\sum_{i,j}\left(\frac{\partial \boldsymbol{\varphi}_i}{\partial t}+\sum_{k=1}^{d}\frac{\partial \boldsymbol{\varphi}_i}{\partial q_k}\dot{q}_k\right)m_{ij}\left(\frac{\partial \boldsymbol{\varphi}_j}{\partial t}+\sum_{l=1}^{d}\frac{\partial \boldsymbol{\varphi}_j}{\partial q_l}\dot{q}_l\right),$$

from which follows that we can represent the kinetic energy in the form

$$T(\mathbf{q}, \dot{\mathbf{q}}, t) = T_0(\mathbf{q}, t) + T_1(\mathbf{q}, \dot{\mathbf{q}}, t) + T_2(\mathbf{q}, \dot{\mathbf{q}}, t),$$

where $T_k(\mathbf{q}, \dot{\mathbf{q}}, t)$ is a homogeneous function of degree k in $\dot{\mathbf{q}}$, namely,

$$T_k(\mathbf{q}, \alpha\dot{\mathbf{q}}, t) = \alpha^k T_k(\mathbf{q}, \dot{\mathbf{q}}, t).$$

In many cases, the Lagrangian has the same form, namely,

$$L(\mathbf{q}, \dot{\mathbf{q}}, t) = L_0(\mathbf{q}, t) + L_1(\mathbf{q}, \dot{\mathbf{q}}, t) + L_2(\mathbf{q}, \dot{\mathbf{q}}, t).$$

Now, for every k,

$$\sum_{j=1}^{d} \dot{q}_j \frac{\partial L_k}{\partial \dot{q}_j} = k\, L_k,$$

from which follows that

$$h(\mathbf{q}, \dot{\mathbf{q}}, t) = \sum_{j=1}^{d} \dot{q}_j \frac{\partial L}{\partial \dot{q}_j} - L = L_2 + L_0.$$

If $\boldsymbol{\varphi}_i$ does not depend on time, then $T = T_2$ and if furthermore, the potential energy does not depend on velocities, $\Phi = L_0$, in which case $h = T + \Phi$. Note that the conservation of h does not require these additional assumptions.

Chapter 5

The two-body central force problem

In this chapter we study in details systems of two point masses in which the only force is an "internal" force of interaction between the two bodies. A notable example for such systems are gravitational systems (e.g., sun and earth).

5.1 Reduction to a one-particle system

Consider two point particles of mass m_1 and m_2. As usual, we denote their positions in $\mathbb{R}^3$ by $\mathbf{r}_1 = (x_1, y_1, z_1)$ and $\mathbf{r}_2 = (x_2, y_2, z_2)$. We assume that the only forces in the system are potential forces derived from a potential function $\Phi(\mathbf{r}_1, \mathbf{r}_2) = g(|\mathbf{r}_1 - \mathbf{r}_2|)$ (i.e. a system satisfying Newton's third law).

This is a six-dimensional system. Yet, we have the choice of selecting convenient generalized coordinates (we don't need constraints as an excuse to switch to convenient variables). Since we know that the center-of-mass plays a distinguished role, we take it for three out of the six degrees of freedom,

$$\boldsymbol{R} = \frac{m_1\mathbf{r}_1 + m_2\mathbf{r}_2}{m_1 + m_2}.$$

The three other coordinates are the ***connector vector***,

$$\mathbf{r} = \mathbf{r}_2 - \mathbf{r}_1.$$

(Note that $(\boldsymbol{R}, \mathbf{r})$ are the generalized coordinates $\mathbf{q}$.) The inverse transformation is

$$\mathbf{r}_1 = \boldsymbol{R} - \frac{m_2}{m_1 + m_2}\mathbf{r} \qquad \text{and} \qquad \mathbf{r}_2 = \boldsymbol{R} + \frac{m_1}{m_1 + m_2}\mathbf{r}.$$

Proceeding with the Lagrangian formulation, we express the kinetic energy in terms of the generalized coordinates,

$$T = \frac{m_1 + m_2}{2}\dot{\boldsymbol{R}}^2 + \frac{m_1 m_2}{2(m_1 + m_2)}\dot{\mathbf{r}}^2.$$

Subtracting the potential energy, the Lagrangian is given by

$$L(\boldsymbol{R}, \mathbf{r}, \dot{\boldsymbol{R}}, \dot{\mathbf{r}}) = \frac{m_1 + m_2}{2}\dot{\boldsymbol{R}}^2 + \frac{m_1 m_2}{2(m_1 + m_2)}\dot{\mathbf{r}}^2 - \Phi(\mathbf{r}).$$

We first observe that the Lagrangian is separated into two terms, one that only depends on $(\boldsymbol{R}, \dot{\boldsymbol{R}})$ and one that only depends on $(\mathbf{r}, \dot{\mathbf{r}})$. Such a Lagrangian is called ***separable***. The huge gain in such case is that the six equations of motion separate into two independent systems of three equations each. That is, we can solve separately for $\boldsymbol{R}(t)$ and for $\mathbf{r}(t)$. This simplification results from the choice of center-of-mass coordinates, along with coordinates that are invariant under translations of the origin.

✎ *Exercise 5.1* What would be a sensible choice of generalized coordinates in a three-body system where the forces are induced only by two-body interactions? Write the Lagrangian of such a system explicitly, as well as the resulting equations of motion. Solve the equations (just kidding!).

The second observation is that $\boldsymbol{R}$ is a cyclic coordinate. Thus, the corresponding equations are trivial,

$$\frac{d}{dt}(m_1 + m_2)\dot{\boldsymbol{R}} = 0,$$

i.e.,

$$\dot{\boldsymbol{R}} = \text{const},$$

which means that the center-of-mass is either at rest or moving with constant speed, namely,

$$\boldsymbol{R}(t) = \boldsymbol{R}(0) + \boldsymbol{V}(0)t.$$

Thus, the entire attention can be turned to the evolution of the connector vector, which is governed by a ***reduced Lagrangian***,

$$L(\mathbf{r}, \dot{\mathbf{r}}) = \frac{m_1 m_2}{2(m_1 + m_2)}\dot{\mathbf{r}}^2 - \Phi(\mathbf{r}).$$

Such a Lagrangian corresponds to a one-particle system with ***reduced mass*** m, where

$$\frac{1}{m} = \frac{1}{m_1} + \frac{1}{m_2}$$

("resistors in parallel"), governed by a conservative force directed along the vector that connects its position to the origin. The Euler-Lagrange equations are

$$m\ddot{\mathbf{r}} + \boldsymbol{\nabla}\Phi(\mathbf{r}) = 0,$$

and they have to be supplemented with initial conditions for $\mathbf{r}$ and $\dot{\mathbf{r}}$.

5.2 Analysis of the reduced one-particle problem

By the previous section, our analysis is restricted to a one-particle system with a ***central force*** derived from a potential $\Phi(\mathbf{r})$. We now observe that the Lagrangian is invariant under any rotation of the axes. As we already know, an invariance results in a constant of motion. Invariance under rotation is related to the conservation of the angular momentum. We can check this directly. For

$$\boldsymbol{L} = \mathbf{r} \times \mathbf{p}$$

we have

$$\frac{d\boldsymbol{L}}{dt} = \mathbf{v} \times \mathbf{p} + \mathbf{r} \times \frac{d\mathbf{p}}{dt} = -\mathbf{r} \times \boldsymbol{\nabla}\Phi.$$

Since we assume that $\Phi(\mathbf{r}) = g(|\mathbf{r}|)$ then

$$\mathbf{r} \times \boldsymbol{\nabla}\Phi = \mathbf{r} \times \left(g'(|\mathbf{r}|) \frac{\mathbf{r}}{|\mathbf{r}|} \right) = 0,$$

i.e., $\boldsymbol{L}$ is conserved. This means, in particular, that the cross product of $\mathbf{r}$ and $\mathbf{v}$ is always in the same direction, i.e, that the motion takes place on a plane passing through the origin. This is a great gain since we can reduce the system into one of only two generalized coordinates.

Even if you don't have this insight, we can get to the same conclusion by using the Lagrangian formalism. We start by changing variables into spherical coordinates, namely,

$$\mathbf{r} = r(\sin\theta\,\cos\phi, \sin\theta\,\sin\phi, \cos\theta).$$

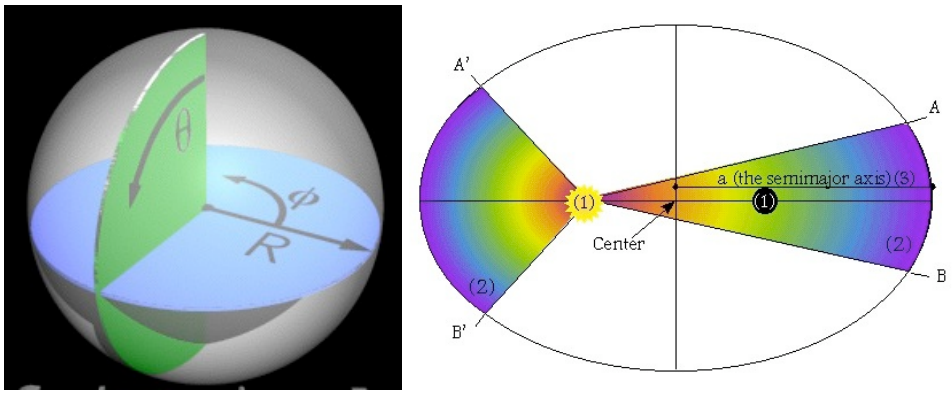


Figure 5.1: Left: spherical coordinates. Right: Kepler's second law or constant areal velocity. The rate at which area is swept by the radius vector is constant in time.

Then the Lagrangian takes the form,

$$L = \frac{m}{2}\left(\dot{r}^2 + r^2\dot{\theta}^2 + r^2\sin^2\theta\,\dot{\phi}^2\right) - g(r).$$

Note that ϕ is a cyclic coordinate, hence

$$p_\phi = mr^2\sin^2\theta\,\dot{\phi}$$

is a constant of motion. Given initial conditions, we can always rotate the axes such that, say, $\dot{\phi}(0) = 0$, i.e., $p_\phi = 0$. Since p_ϕ is conserved, it follows that the "longitude" ϕ remains constant in time, i.e., the motion is on a plane with polar coordinates (r, θ). This, at least, will allows us to draw two-dimensional pictures...

The equation for θ is then

$$p_\theta = mr^2\dot{\theta} = \text{const.}$$

The first law we have deduced is that motion takes place on a plane. The second law is that $r^2\dot{\theta}$ is constant. This quantity is the ***areal velocity*** of the particle—the rate at which area is swept by the position vector. This quantity is thus constant in time. This law is known as ***kepler's second law***. Note that it does not depend on the precise potential. The conservation of angular momentum is a consequence of the force field being central (directed toward the origin). Kepler's two other laws are pertinent to the inverse square gravitational force, and we will return to them when we address this particular example.

Figure 5.2: Johannes Kepler (1571–1630)

Remains the equation for r. The Euler-Lagrange equation is

$$m\ddot{r} - mr\dot{\theta}^2 + g'(r) = 0.$$

We can however substitute the constant of motion p_θ to get a closed equation for $r(t)$:

$$m\ddot{r} - \frac{p_\theta^2}{mr^3} + g'(r) = 0.$$

Can we solve this equation? It depends on the potential g. Yet, we can proceed further but using the conservation of energy. Multiplying the equation by $\dot{r}$ we obtain,

$$\frac{d}{dt}\left[\frac{m}{2}\dot{r}^2 + \frac{p_\theta^2}{2mr^2} + g(r)\right] = 0,$$

i.e.,

$$E = \frac{m}{2}\dot{r}^2 + \frac{p_\theta^2}{2mr^2} + g(r)$$

is yet another constant of motion. This means that we can reduce the system into a first order equation,

$$\frac{dr}{dt} = \pm\sqrt{\frac{2}{m}}\sqrt{E - g(r) - \frac{p_\theta^2}{2mr^2}}.$$

Suppose we start with an initial condition where $dr/dt > 0$. Then it won't change sign without crossing zero first, and we can integrate to get

$$t - t_0 = \sqrt{\frac{m}{2}} \int_{r(t_0)}^{r(t)} \frac{du}{\sqrt{E - g(u) - p_\theta^2/2mu^2}}.$$

In certain cases, this integral can be computed analytically and the relation between r and t can be inverted. In either case, we have reduced the original problem into the computation of an integral, which can easily be approximated by quadratures.

Once $r(t)$ has been calculated (either exactly or approximately), we obtain $\theta(t)$ by

$$\theta(t) - \theta(t_0) = \frac{p_\theta}{m} \int_{t_0}^{t} \frac{ds}{r^2(s)}.$$

In a later section we will solve these integrals for specific choices of potential functions.

5.3 Classification of orbits

Even without an analytic solution, a lot can be said *qualitatively* on the nature of those solutions. We start from the equation for r,

$$m\ddot{r} - \frac{p_\theta^2}{mr^3} + g'(r) = 0.$$

Although this equation was derived from an equation of motion in the plane, we can interpret it as an equation for a "fictitious" particle of mass m, moving on the line under the influence of an ***effective potential***,

$$G(r) = g(r) + \frac{p_\theta^2}{2mr^2},$$

where p_θ is fixed once we know the initial conditions of the original system.

What we are doing here is common practice in physics: we identify a set of equations as that of a different system, and use then the knowledge and intuition acquired from the other analogous system. Indeed, equations are equations, regardless of the physical system they were derived from. In this case, the solution $r(t)$ is

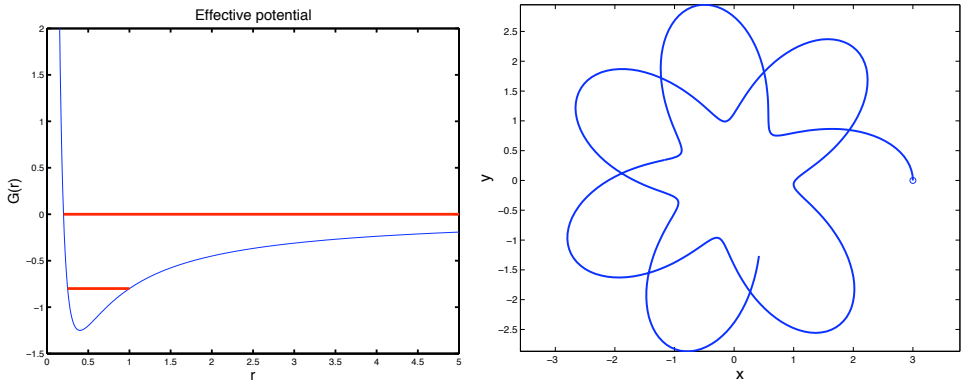


Figure 5.3: Left: the effective potential $G(r)$. Right: a non-closed trajectory in (x, y) plane.

the same as the trajectory of a particle moving frictionless under the influence of the potential function $G(r)$. We have already made use of the energy conservation,

$$E = \frac{m\dot{r}^2}{2} + G(r) = \text{const.}$$

We are now going to make use of more of this insight to determine properties of this trajectory.

Consider Figure 5.3 (left), which corresponds to the case $g(r) = -1/r$ and $p_\theta = \sqrt{2}$. The characteristics of this potential are a positive blowup at the origin and a decay to zero at infinity. Suppose that the energy (determined by the initial data) is negative (the lower red line). Then, by energy conservation the particle is confined in a finite range of radii, $r \in [r_1, r_2]$. The motion in r will be periodic in time going between the two extreme values, where the radial velocity vanishes, and the motion is inverted; the trajectory is then *bounded*. As explained above, we are fully allowed to draw conclusions from the mechanical analog of a bead moving under the only influence of gravity and a track that has this shape. Note that when we revert to the (r, θ) picture, there is no guarantee that the planar motion will form a closed trajectory; see Figure 5.3 (right).

Conversely, if the energy is positive, then if $\dot{r}$ is initially negative, the particle will approach the origin until it hits the potential wall, turns back, and goes all the way to infinity. That is, the trajectory is ***unbounded***.

A third possibility is then $G(r) \to -\infty$ as $r \to 0$. In such case there could be

trajectories that are attracted toward the origin with ever increasing speed. Such systems are in a sense singular.

✎ *Exercise 5.2* A particle moves in a central force field with potential

$$g(r) = -\frac{e^{-r}}{r}.$$

Discuss the nature of the possible solutions as function of the angular momentum p_θ and the energy E.

5.4 Orbit equations

Rather than looking for the time evolution of the system, $(r(t), \theta(t))$, we could try and find directly the ***orbit*** of the motion, i.e., $r(\theta)$. In such a description, time is absent, although it can always be recovered from the relation,

$$p_\theta = mr^2\dot{\theta},$$

i.e.,

$$t_1 - t_0 = \int_{\theta_0}^{\theta_1} \frac{mr^2(\theta)}{p_\theta}\, d\theta.$$

Recall that the equations of motion for $r(t)$ are

$$m\frac{d^2r}{dt^2} - \frac{p_\theta^2}{mr^3} + g'(r) = 0.$$

If we express r as function of θ, then

$$\frac{dr}{dt} = \frac{d\theta}{dt}\frac{dr}{d\theta} = \frac{p_\theta}{mr^2}\frac{dr}{d\theta},$$

and

$$\frac{d^2r}{dt^2} = \frac{p_\theta}{mr^2}\frac{d}{d\theta}\left(\frac{p_\theta}{mr^2}\frac{dr}{d\theta}\right),$$

hence we have

$$m\frac{p_\theta}{mr^2}\frac{d}{d\theta}\left(\frac{p_\theta}{mr^2}\frac{dr}{d\theta}\right) - \frac{p_\theta^2}{mr^3} + g'(r) = 0.$$

It is useful to change the dependent variable, $u = 1/r$. Then,

$$\frac{dr}{d\theta} = -\frac{1}{u^2}\frac{du}{dr},$$

and we get

$$-m\frac{p_\theta}{m}u^2\frac{d}{d\theta}\left(\frac{p_\theta}{m}\frac{du}{d\theta}\right) - \frac{p_\theta^2}{m}u^3 + g'\left(\frac{1}{u}\right) = 0,$$

and further

$$\frac{d^2u}{d\theta^2} + u - \frac{m}{p_\theta^2}\frac{1}{u^2}g'\left(\frac{1}{u}\right) = 0. \tag{5.1}$$

In general, Equation (5.1) cannot be solved. A class of potentials g for which explicit solutions (in terms of special functions) exists are power-law potentials.

5.5 Gravitational systems

We now turn to the particular case of gravitational systems. The potential is

$$g(r) = -\frac{\alpha}{r},$$

where α is a constant that depends on the universal gravitational constant and the masses of the two particles. Thus, $g'(r) = \alpha/r^2$, which substituted into (5.1) yields the orbit equation

$$\frac{d^2u}{d\theta^2} + u - \frac{m\alpha}{p_\theta^2} = 0.$$

This equation has the very simple solution,

$$u(\theta) = \frac{m\alpha}{p_\theta^2}\left[1 + A\,\cos(\theta - \theta_0)\right],$$

where A, θ_0 are constants of integration. Reverting to the original variables,

$$\frac{1}{r(\theta)} = \frac{m\alpha}{p_\theta^2}\left[1 + A\,\cos(\theta - \theta_0)\right].$$

We would like to connect the constant of integration to the energy and angular momentum of the system. We have

$$\frac{dr}{dt} = \frac{p_\theta}{mr^2}\frac{dr}{d\theta} = -\frac{p_\theta}{m}\frac{du}{d\theta} = \frac{\alpha}{p_\theta}A\sin(\theta - \theta_0).$$

Also,

$$G(r) = -\alpha u + \frac{p_\theta^2}{2m}u^2 = -\frac{m\alpha^2}{p_\theta^2}\left[1 + A\,\cos(\theta - \theta_0)\right] + \frac{m\alpha^2}{2p_\theta^2}\left[1 + A\,\cos(\theta - \theta_0)\right]^2 .$$

The total energy is therefore

$$E = \frac{m\alpha^2 A^2}{2p_\theta^2}\sin^2(\theta - \theta_0) + \frac{m\alpha^2 A^2}{2p_\theta^2}\cos^2(\theta - \theta_0) - \frac{m\alpha^2}{2p_\theta^2} = \frac{m\alpha^2}{2p_\theta^2}\left(A^2 - 1\right).$$

Inverting this relation, we get

$$A = \sqrt{1 + \frac{2p_\theta^2 E}{m\alpha^2}}.$$

To conclude, we have obtained the following orbit,

$$\frac{1}{r} = \frac{m\alpha}{p_\theta^2}\left[1 + \sqrt{1 + \frac{2p_\theta^2 E}{m\alpha^2}}\,\cos(\theta - \theta_0)\right].$$

What can be said about an orbit of the form

$$\frac{1}{r} = C[1 + \epsilon\,\cos(\theta - \theta_0)].$$

The simplest case is when $\epsilon = 0$, in which case r is constant, i.e., motion along a circle. This corresponds to the case where

$$E = -\frac{m\alpha^2}{2p_\theta^2},$$

which coincides with the minimum of the fictitious potential

$$G(r) = -\frac{\alpha}{r} + \frac{p_\theta^2}{2mr^2}.$$

More generally, we claim that the orbits are always ***conic sections***. Indeed, set

$$r = \sqrt{x^2 + y^2} \qquad \text{and} \qquad \tan(\theta - \theta_0) = \frac{y}{x},$$

and from the latter we get

$$\cos^2(\theta - \theta_0) = \frac{1}{1 + \tan^2(\theta - \theta_0)} = \frac{1}{1 + y^2/x^2} = \frac{x^2}{x^2 + y^2}.$$

Then,

$$\frac{1}{\sqrt{x^2 + y^2}} = C\left[1 + \epsilon\frac{x}{\sqrt{x^2 + y^2}}\right],$$

which we can further manipulate into

$$1 - \epsilon C x = C\sqrt{x^2 + y^2} \qquad \Rightarrow \qquad 1 - \epsilon C x + \epsilon^2 C^2 x^2 = C^2(x^2 + y^2).$$

The next simple case is when $\epsilon = 1$, in which case

$$1 - Cx = C^2 y^2,$$

which means that the trajectory is a parabola. Energy-wise this case corresponds to the critical value $E = 0$. Remain the cases of $0 < \epsilon < 1$ and $\epsilon > 1$. The first case corresponds to an ellipse (i.e., a closed trajectory), whereas the second case corresponds to an hyperbola (i.e., an unbounded trajectory).

✎ *Exercise 5.3* Kepler's third law asserts that the period τ of the motion and the main radius a of the ellipse satisfy a relation

$$\tau = c\, a^{3/2},$$

where c is a constant independent of the initial data. Figure out how to prove it.

Chapter 6

Small oscillations

6.1 Equilibria and deviations

A mechanical system is said to be at ***equilibrium*** if its configuration $\mathbf{q}$ is stationary in time, i.e., $(\mathbf{q}, \dot{\mathbf{q}} = 0)$ is a ***fixed point*** of the Euler-Lagrange equations. For a single (unconstrained) particle in a potential field $\Phi(\mathbf{r})$, the equations of motion are

$$m\ddot{\mathbf{r}} = -\boldsymbol{\nabla}\Phi(\mathbf{r}),$$

hence an equilibrium is a point $\mathbf{r}$ where $\boldsymbol{\nabla}\Phi(\mathbf{r}) = 0$. More generally, suppose that the Lagrangian of the system is of the (quite general) form

$$L(\mathbf{q}, \dot{\mathbf{q}}) = \frac{1}{2}\sum_{i,j=1}^{d} a_{ij}(\mathbf{q})\dot{q}_i\dot{q}_j - \Phi(\mathbf{q}),$$

then an equilibrium is a configuration $\mathbf{q}$ such that $\boldsymbol{\nabla}\Phi(\mathbf{q}) = 0$, or componentwise,

$$\frac{\partial\Phi}{\partial q_i}(\mathbf{q}) = 0, \qquad i = 1, \ldots, d.$$

*Definition 6.1 An equilibrium point $\mathbf{q}^{eq}$ is called **stable** if a small initial deviation about it results in a motion that remains close to it for all times. Formally, for every $\epsilon > 0$ there exists a $\delta > 0$ such that*

$$|\mathbf{q}(0) - \mathbf{q}^{eq}| < \delta \qquad \Rightarrow \qquad |\mathbf{q}(\mathbf{t}) - \mathbf{q}^{eq}| < \epsilon \text{ for all } t.$$

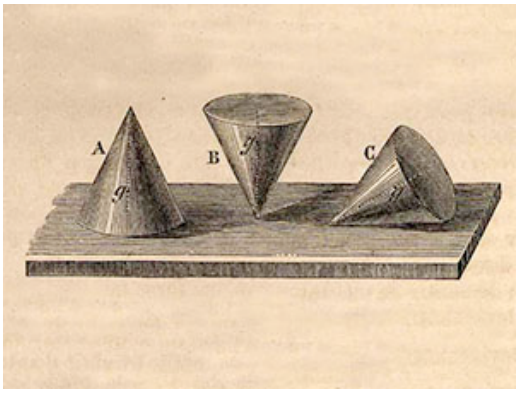


Figure 6.1: Stable, unstable and indifferent equilibria

Comment: The system cannot tend asymptotically to the rest state in the absence of friction. It will rather oscillate, which is precisely the subject of this chapter.

Let $\mathbf{q}^{\mathrm{eq}}$ then be an equilibrium point, and define

$$\mathbf{q} = \mathbf{q}^{\mathrm{eq}} + \boldsymbol{\eta}.$$

Taylor expanding the kinetic and potential energies about the equilibrium point we get

$$T = \frac{1}{2}\sum_{i,j=1}^{d} \underbrace{a_{ij}(\mathbf{q}^{\mathrm{eq}})}_{m_{ij}} \dot{\eta}_i \dot{\eta}_j + O(\dot{\eta}^2 \eta)$$

$$\Phi = \Phi\,(\mathbf{q}^{\mathrm{eq}}) + \frac{1}{2}\sum_{i,j=1}^{d} \underbrace{\frac{\partial^2 \Phi}{\partial q_i\, \partial q_j}(\mathbf{q}^{\mathrm{eq}})}_{v_{ij}} \eta_i \eta_j + O(\eta^3).$$

The coefficient Φ_{ij} are symmetric with respect to i, j; the coefficients m_{ij} can be symmetrized without affecting the double sum, hence we will assume that $m_{ij} = m_{ji}$.

Substituting into the equations of motions we get

$$\sum_{j=1}^{d} m_{ij}\ddot{\eta}_j + \sum_{j=1}^{d} v_{ij}\eta_j = O(\eta^2).$$

Assuming that the right hand side can be neglected, this is a linear system with constant coefficients—something we learned extensively in the ODE course.

6.2 Normal mode equations

Denote by M, V the matrices with coefficients m_{ij}, v_{ij}. The linear system can then be written in the form

$$M\ddot{\boldsymbol{\eta}} + V\boldsymbol{\eta} = 0.$$

We first claim that the matrix M must be symmetric positive-definite; this is a physical claim that requires the kinetic energy to be always non-negative. In particular, it is invertible and we can write

$$\ddot{\boldsymbol{\eta}} = -M^{-1}V\boldsymbol{\eta}.$$

Let S be an invertible matrix and define

$$\boldsymbol{z} = S\boldsymbol{\eta}.$$

Substituting into the linear system we get

$$\ddot{\boldsymbol{z}} = -S\,M^{-1}VS^{-1}\boldsymbol{z}.$$

If the matrix $M^{-1}V$ is diagonalizable, then we would take S to be the diagonalizing transformation, in which case we end with a diagonal system,

$$\ddot{\boldsymbol{z}} = -\Lambda\boldsymbol{z}.$$

We call each of the transformed coordinates z_i a ***normal coordinate***. All the normal coordinates oscillate in time (hence the η's too) if all the diagonal entries of Λ are real and positive.

Since M is symmetric positive-definite it has a square-root, and we can write

$$\Lambda = (S\,M^{-1/2})M^{-1/2}VM^{-1/2}(S\,M^{-1/2})^{-1},$$

and therefore

$$\mathrm{ev}\,\Lambda = \mathrm{ev}\,(M^{-1/2}VM^{-1/2}).$$

The right-hand side is a symmetric matrix, hence all its eigenvalues are real. The question is underwhat conditions all the eigenvalues are positive.

Proposition 6.1 The matrix $M^{-1/2}VM^{-1/2}$ is positive definite if and only if V is such.

Proof: This is immediate from the fact that $M^{-1/2}$ is one-to-one and onto. For example, if V is symmetric positive-definite then for every $0 \neq \boldsymbol{x} \in \mathbb{R}^n$,

$$\boldsymbol{x}^T M^{-1/2} V M^{-1/2} \boldsymbol{x} = (M^{-1/2}\boldsymbol{x})^T V (M^{-1/2}\boldsymbol{x}) > 0.$$

■

Thus we have obtained an expected result. The equilibrium point is stable if the potential Φ is a local minimum. Small amplitude motion about this equilibrium consists of a combination of oscillations,

$$z_i(t) = z_i(0)\, \cos(\sqrt{\lambda_i}t) + \frac{\dot{z}_i(0)}{\sqrt{\lambda_i}}\, \sin(\sqrt{\lambda_i}t).$$

(Clearly, if the $\boldsymbol{z}$'s oscillate so do the $\boldsymbol{\eta}s$.)

6.3 Oscillations of a tri-atomic molecule

Consider the following model of a tri-atomic molecule. Three atoms of masses m, μ, m arranged on a line, and connected by linear springs of rest length b and spring constant k. In this model, if x_1, x_2, x_3 denote the positions of the atoms on the line, then the Lagrangian is

$$L(\mathbf{x}, \dot{\mathbf{x}}) = \frac{1}{2}\left(m\dot{x}_1^2 + \mu\dot{x}_2^2 + m\dot{x}_3^2\right) - \frac{k}{2}(x_2 - x_1 - b)^2 - \frac{k}{2}(x_3 - x_2 - b)^2.$$

Let x_1^0, $x_2^0 = x_1^0 + b$ and $x_3^0 = x_2^0 + b$, and consider the following deviations,

$$\mathbf{x} = \mathbf{x}^0 + \boldsymbol{\eta}.$$

The Lagrangian takes then the form

$$L(\boldsymbol{\eta}, \dot{\boldsymbol{\eta}}) = \frac{1}{2}\left(m\dot{\eta}_1^2 + \mu\dot{\eta}_2^2 + m\dot{\eta}_3^2\right) - \frac{k}{2}(\eta_2 - \eta_1)^2 - \frac{k}{2}(\eta_3 - \eta_2)^2.$$

The matrices M, V are therefore

$$M = \begin{pmatrix} m & 0 & 0 \\ 0 & \mu & 0 \\ 0 & 0 & m \end{pmatrix} \qquad \text{and} \qquad V = k\begin{pmatrix} 1 & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 1 \end{pmatrix}.$$

Thus, the normal frequencies of the system are the eigenvalues of the matrix

$$M^{-1/2}VM^{-1/2} = k\begin{pmatrix} 1/m & -1/\sqrt{m\mu} & 0 \\ -1/\sqrt{m\mu} & 2/\mu & -1/\sqrt{m\mu} \\ 0 & -1/\sqrt{m\mu} & 1/m \end{pmatrix}.$$

If we define $\omega = \sqrt{k/m}$ and $\Omega = \sqrt{k/\mu}$, then

$$M^{-1/2}VM^{-1/2} = \begin{pmatrix} \omega^2 & -\omega\Omega & 0 \\ -\omega\Omega & 2\Omega^2 & -\omega\Omega \\ 0 & -\omega\Omega & \omega^2 \end{pmatrix}.$$

The eigenvalues solve the cubic equation

$$(\omega^2 - \lambda)\left[(2\Omega^2 - \lambda)(\omega^2 - \lambda) - 2\omega^2\Omega^2\right] = 0,$$

i.e.,

$$\lambda_1 = \omega^2 \qquad \lambda_2 = 0 \qquad \lambda_3 = \omega^2 + 2\Omega^2.$$

The zero eigenvalue can seem surprising until we recognize that a possible mode of motion is translation (i.e., no oscillations). That is,

$$\eta(t) = \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}(1 + \alpha t)$$

is a solution of this system. It is easy to see what the two other frequencies correspond to. We can do it formally by finding the diagonalizing transformation. We can also guess the solutions. For example, if we set $\eta_1 = -\eta_3$ and $\eta_2 = 0$, then

$$\eta_1(t) = \eta_1(0)\cos(\sqrt{\lambda_1}t + \theta_0).$$

The other eigenmode corresponds to a motion with $\eta_1 = \eta_3$ and $2m\eta_1 = -M\eta_2$, in which case we get

$$\eta_1(t) = \eta_1(0)\cos(\sqrt{\lambda_2}t + \theta_0).$$

The most general motion is a combination of the three eigenmodes,

$$\boldsymbol{\eta}(t) = a_1\begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix}\cos(\omega t + \theta_1) + a_2\begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}(1 + \alpha t) + a_3\begin{pmatrix} 1 \\ -2m/M \\ 1 \end{pmatrix}\cos(\sqrt{\omega^2 + 2\Omega^2}t + \theta_3).$$

✎ *Exercise 6.1* Consider a 5-atomic linear molecule with masses m, μ, m, μ, m and spring constants k. What can you say about the oscillations of such a molecule about its equilibrium configuration?

Example: Oscillation of the central-force system

$$L(r, \dot{r}) = \frac{m}{2}\dot{r}^2 - G(r),$$

for

$$G(r) = -\frac{\alpha}{r} + \frac{p_\theta^2}{2mr^2},$$

about the equilibrium point

$$r_{eq} = \frac{p_\theta^2}{m\alpha}.$$

One gets oscillations with frequency that is exactly the frequency of the rotations in θ, which implies a closed trajectory. Indeed, the actual trajectory is an ellipse. ▲

Chapter 7

Hamiltonian mechanics

7.1 The Legendre transformation

Consider a real-valued convex function $f : \mathbb{R} \to \mathbb{R}$; altough this is not a necessity, we will asume f to be twice differentiable, i.e., $\partial^2 f/\partial x^2(x) > 0$.

Given such a function f, we define a new function, $f^* : \mathbb{R} \to \mathbb{R}$, as follows,

$$f^*(p) = \max_{x \in \mathbb{R}} (px - f(x)).$$

We can make this definition more explicit since f is assumed to be differentiable. For every p the maximum of $px - f(x)$ is obtained for an x satisfying $p - f'(x) = 0$, so that

$$f^*(p) = px(p) - f(x(p)),$$

where $x(p)$ stands for the solution of $f'(x) = p$, or $x(p) = (f')^{-1}(p)$. The function $x(p)$ is indeed well-defined if f is convex.

The function f^* is called the ***Legendre transform*** of f; it has a simple geometric interpretation. Interpret p as the slope of a tangent to the graph of f, and suppose that the point of tangency is $(x_0, f(x_0))$. The equation of this tangent is

$$y(x) = f(x_0) + p(x - x_0).$$

Since $f'(x_0) = p$, then $x_0 = x(p)$, and the intersection of the tangent line with the y axis is at the point

$$f(x_0) - px_0 = f(x(p)) - px(p) = -f^*(p).$$

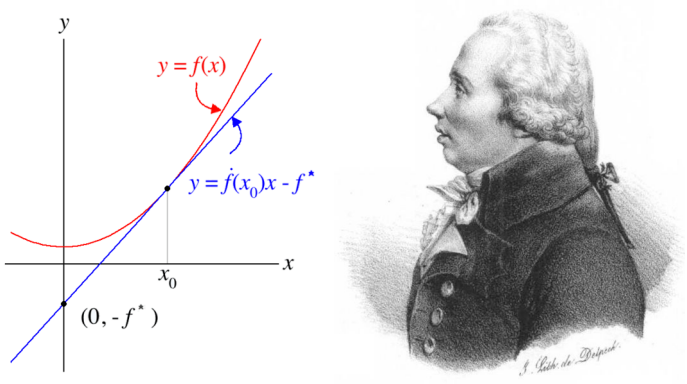


Figure 7.1: Left: the Legendre transformation: the graph in red is $f(x)$. Its tangent with slope p intersects the y-axis at the point $-f^*(p)$. Right: Adrien-Marie Legendre (1752–1833).

The function f^* "encodes" the same information as f, through its tangents. Given the slope p of the tangent, $f^*(p)$ is (up to a sign) the intersection with the y-axis. The knowledge of $f^*(p)$ lets us reconstruct the original function $f(x)$ as the "envelop" of tangent lines.

How do we actually recover $f(x)$ given $f^*(p)$? We now show that the Legendre transform is its own inverse. Indeed,

$$f^{**}(s) = s\,[(f^*)']^{-1}(s) - f^*([(f^*)']^{-1}(s)), \tag{7.1}$$

whereas

$$f^*(p) = p\,(f')^{-1}(p) - f((f')^{-1}(p)).$$

Thus,

$$(f^*)'(p) = (f')^{-1}(p) + p((f')^{-1})'(p) - \underbrace{f'((f')^{-1})(p)}_{p}((f')^{-1})'(p).$$

The last two terms cancel, hence

$$(f^*)'(p) = (f')^{-1}(p), \qquad \text{and} \qquad [(f^*)']^{-1} = f'. \tag{7.2}$$

Furthermore,

$$f^*(f'(s)) = f'(s)\,\underbrace{(f')^{-1}(f'(s))}_{s} - f(\underbrace{(f')^{-1}(f'(s))}_{s}) = s\,f'(s) - f(s), \tag{7.3}$$

Figure 7.2: William Rowan Hamilton (1805–1865).

hence substituting (7.2) and (7.3) into (7.1),

$$f^{**}(s) = s[(f')^{-1}]^{-1}(s) - f^*(f'(s)) = s\,f'(s) - [s\,f'(s) - f(s)] = f(s).$$

The Legendre transform can be easily generalized to higher dimension. We will see an application of it in the next section.

✎ *Exercise 7.1* Find the Legendre transform of the function e^x.

✎ *Exercise 7.2* Show that the Legendre transform satisfies the following algebraic properties:

1. $f(x) = a\,g(x) \quad \Rightarrow \quad f^*(p) = a\,g^*(p/a)$.
2. $f(x) = g(ax) \quad \Rightarrow \quad f^*(p) = g^*(p/a)$.
3. $f(x) = g(x+b) \quad \Rightarrow \quad f^*(p) = g^*(p) - b$.
4. $f(x) = g^{-1}(x) \quad \Rightarrow \quad f^*(p) = -p\,g^*(1/p)$.

7.2 Hamilton's equations

Let's start with a short summary of the Lagrangian formulation of the laws of mechanics. The state of a mechanical system is described by a vector $\mathbf{q} \subseteq \mathbb{R}^n$,

a point in ***configuration space***. The time evolution of the configuration, i.e., the path $\mathbf{q}(t) : \mathbb{R} \to \mathbb{R}^n$, is governed by a second-order differential system,

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}_i}\right) - \frac{\partial L}{\partial q_i} = 0, \qquad i = 1, \ldots, n.$$

For simplicity, let's restrict ourselves to $n = 1$, which will mainly save us some indexation. Recall also that the Lagrange equations can be derived from a variational principle, whereby the path $q(t)$ is one for which the action functional

$$I[q] = \int_{t_1}^{t_2} L(q(t), \dot{q}(t), t)\, dt$$

is minimal among all paths that satisfy end conditions $q(t_1)$ and $q(t_2)$.

In my own effort to parse Chapter 8 of Goldstein, I reached the conclusion that the notation $\dot{q}$ is more confusing than helpful. Sometimes we think of $\dot{q}$ as the name of a variable and sometimes as the time derivative of a function $q(t)$. To avoid such a confusion, let's reformulate Lagrangian mechanics as follows: the Lagrangian is a function of three variables, $L = L(q, z, t)$. The laws of mechanics are a second-order equation for the path $q(t)$,

$$-\frac{d}{dt}\left[\frac{\partial L}{\partial z}\left(q(t), \frac{dq(t)}{dt}, t\right)\right] + \frac{\partial L}{\partial q}\left(q(t), \frac{dq(t)}{dt}, t\right) = 0.$$

As is standard practice, this second-order equation can be turned into a set of two first-order equations by

$$\begin{aligned} &\frac{dq}{dt} = z \\ &\frac{d}{dt}\left[\frac{\partial L}{\partial z}(q, z, t)\right] - \frac{\partial L}{\partial q}(q, z, t) = 0. \end{aligned}$$

We defined the momentum conjugate to the coordinate q as

$$p = \frac{\partial L}{\partial z}(q, z, t).$$

Thus, we view p as a function of (q, z, t).

In the Hamiltonian formulation of the laws of mechanics, we describe the state of the system with the pair of variable (q, p) (the set of points (q, p) is called the

phase space). Thus, we need to change variables and rewrite the equations of motions as equations for the functions $q(t)$, $p(t)$. The question is how to do it.

The Lagrangian is a function of two variables q and z (and possibly time). Consider the Legendre transformation of the Lagrangian with respect to the variable z,

$$L^*(q, p, t) = p\, z(q, p, t) - L(q, z(q, p, t), t),$$

where $z(q, p, t)$ is the inverse relation to

$$p = \frac{\partial L}{\partial z}(q, z, t),$$

i.e., it is precisely our definition of the conjugate momentum. The Legendre transformation of the Lagrangian is called the ***Hamiltonian***, and it is commonly denoted by the letter H,

$$H(q, p, t) = p\, z(q, p, t) - L(q, z(q, p, t), t).$$

We now examine the derivatives of H with respect to its arguments. First,

$$\frac{\partial H}{\partial q}(q, p, t) = p\frac{\partial z}{\partial q}(q, p, t) - \frac{\partial L}{\partial q}(q, z(q, p, t), t) - \frac{\partial L}{\partial z}(q, z(q, p, t), t)\frac{\partial z}{\partial q}(q, p, t).$$

However the first and the third term cancel, so that

$$\frac{\partial H}{\partial q}(q, p, t) = -\frac{\partial L}{\partial q}(q, z(q, p, t), t).$$

Second,

$$\frac{\partial H}{\partial p}(q, p, t) = z(q, p, t) + p\frac{\partial z}{\partial p}(q, p, t) - \frac{\partial L}{\partial z}(q, z(q, p, t), t)\frac{\partial z}{\partial p}(q, p, t).$$

Again, we have a cancellation, so that

$$\frac{\partial H}{\partial p}(q, p, t) = z(q, p, t).$$

So far, no dynamics; just relations between functions. Now, we evaluate those relations along the path, $q(t)$, $p(t)$. The Lagrange equations give us

$$z(q(t), p(t), q) = \frac{dq(t)}{dt},$$

and

$$-\frac{\partial L}{\partial q}(q(t), z(q(t), p(t), t), t) = \frac{dp(t)}{dt}.$$

Thus ***Hamilton's equations*** are

$$\frac{dq}{dt} = \frac{\partial H}{\partial p}(q, p, t) \qquad \frac{dp}{dt} = -\frac{\partial H}{\partial q}(q, p, t)$$

This procedure can easily be extended to vector-valued $\mathbf{q}$. Given the Lagrangian $L(\mathbf{q}, z, t)$ we define the Hamiltonian,

$$H(\mathbf{q}, \mathbf{p}, t) = \sum_{i=1}^{n} p_i z_i(\mathbf{q}, \mathbf{p}, t) - L(\mathbf{q}, z(\mathbf{q}, \mathbf{p}, t), t),$$

where the transformation between $(\mathbf{q}, z, t)$ and $(\mathbf{q}, \mathbf{p}, t)$ is

$$p_i = \frac{\partial L}{\partial z_i}(\mathbf{q}, z, t).$$

Hamilton's equations are a system of $2n$ first-order equations

$$\begin{aligned} \frac{dq_i}{dt} &= \frac{\partial H}{\partial p_i}(\mathbf{q}, \mathbf{p}, t) \\ \frac{dp_i}{dt} &= -\frac{\partial H}{\partial q_i}(\mathbf{q}, \mathbf{p}, t). \end{aligned} \tag{7.4}$$

So what does it take to apply Hamilton's formalism?

1. Choose the generalized coordinates $\mathbf{q}$ and construct the Lagrangian $L(\mathbf{q}, \dot{\mathbf{q}}, t)$.
2. Invert the relations
$$p_i = \frac{\partial L}{\partial \dot{q}_i}(\mathbf{q}, \dot{\mathbf{q}}, t)$$
to express $\dot{\mathbf{q}}$ as a function of $(\mathbf{q}, \mathbf{p}, t)$.
3. Construct the Hamiltonian H as a function of $(\mathbf{q}, \mathbf{p}, t)$.
4. Derive Hamilton's equations of motion.

Example: Consider a free particle in one-dimension, whose Lagrangian is

$$L(q, \dot{q}, t) = \frac{m}{2}\dot{q}^2.$$

The momentum conjugate to q is

$$p = \frac{\partial L}{\partial \dot{q}} = m\dot{q},$$

i.e., $\dot{q} = p/m$. The Hamiltonian is correspondingly

$$H(q, p) = p\dot{q} - L = \frac{p^2}{2m}.$$

Note that the Lagrangian and the Hamiltonian assume the same values (both equal to the kinetic energy). They are however different functions since they depend on different variables.

Finally, the equations of motion are

$$\frac{dq}{dt} = \frac{\partial H}{\partial p} = \frac{p}{m} \qquad \text{and} \qquad \frac{dp}{dt} = -\frac{\partial H}{\partial q} = 0,$$

so that p is a constant of motion and

$$q(t) = q(0) + \frac{p}{m}t.$$

▲

Example: The next example is that of a mass in a central force field. If we use spherical coordinates, the Lagrangian is

$$L(r, \theta, \phi, \dot{r}, \dot{\theta}, \dot{\phi}) = \frac{m}{2}(\dot{r}^2 + r^2\dot{\theta}^2 + r^2 \sin^2\theta\dot{\phi}^2) - g(r),$$

where g is the central potential. Introducing the generalize momenta,

$$p_r = m\dot{r} \qquad p_\theta = mr^2\dot{\theta} \quad \text{and} \quad p_\phi = mr^2 \sin^2\theta\dot{\phi},$$

we obtain that the Hamiltonian is

$$H(r, \theta, \phi, p_r, p_\theta, p_\phi) = \frac{1}{2m}\left(p_r^2 + \frac{p_\theta^2}{r^2} + \frac{p_\phi^2}{r^2 \sin^2\theta}\right) + g(r).$$

Hamilton's equations are

$$\begin{aligned}
\frac{dr}{dt} &= \frac{p_r}{m} & \frac{dp_r}{dt} &= \frac{p_\theta^2}{mr^3} + \frac{p_\phi^2}{mr^3 \sin^2\theta} \\
\frac{d\theta}{dt} &= \frac{p_\theta}{mr^2} & \frac{dp_\theta}{dt} &= \frac{p_\phi^2 \cos\theta}{mr^2 \sin^3\theta} \\
\frac{d\phi}{dt} &= \frac{p_\phi}{mr^2 \sin^2\theta} & \frac{dp_\phi}{dt} &= 0.
\end{aligned}$$

From here we get at once that p_ϕ is conserved (could well be zero) and therefore p_θ is conserved (etc.). ▲

Hamiltonian and energy Those of you with good memory may have recognized the quantity

$$\sum_{i=1}^{n} p_i \frac{dq_i}{dt} - L\left(\mathbf{q}, \frac{d\mathbf{q}}{dt}, t\right),$$

as the total mechanical energy, $T + \Phi$, which is conserved if the Lagrangian does not depend on time explicitly. To be more precise, the identification of this function as the total energy and its conservation under the law of mechanics are two separate issues.

The conservation of the Hamiltonian when it is time-independent follows at once from Hamilton's equations,

$$\frac{d}{dt}H(\mathbf{q}(t), \mathbf{p}(t), t) = \sum_{i=1}^{n}\left(\frac{\partial H}{\partial q_i}\frac{dq_i}{dt} + \frac{\partial H}{\partial p_i}\frac{dp_i}{dt}\right) + \frac{\partial H}{\partial t} = \frac{\partial H}{\partial t},$$

so that H is conserved if $\partial H/\partial t = 0$. The identification of the Hamiltonian with energy requires the relation between the Cartesian coordinate $\mathbf{r}_i$ and the generalized coordinate $\mathbf{q}$ to be time-independent,

$$\mathbf{r}_1 = \boldsymbol{\varphi}_i(\mathbf{q}),$$

as well as the potential energy not to depend on the generalized velocities, $\Phi = \Phi(\mathbf{q})$. Then,

$$\dot{\mathbf{r}}_i = \sum_{j=1}^{d} \frac{\partial \boldsymbol{\varphi}_i}{\partial q_j}\dot{q}_j,$$

i.e.,

$$|\dot{\mathbf{r}}_i|^2 = \sum_{j,k=1}^{d} \frac{\partial \boldsymbol{\varphi}_i}{\partial q_j} \cdot \frac{\partial \boldsymbol{\varphi}_i}{\partial q_k}\dot{q}_j\dot{q}_k,$$

from which we get

$$L(\mathbf{q}, \dot{\mathbf{q}}) = \frac{1}{2}\sum_{i=1}^{n} m_i \sum_{j,k=1}^{d} \frac{\partial \boldsymbol{\varphi}_i}{\partial q_j} \cdot \frac{\partial \boldsymbol{\varphi}_i}{\partial q_k}\dot{q}_j\dot{q}_k - \Phi(\mathbf{q}).$$

The momentum conjugate to q_j is then

$$p_j = \sum_{i=1}^{n} m_i \sum_{k=1}^{d} \frac{\partial \boldsymbol{\varphi}_i}{\partial q_j} \cdot \frac{\partial \boldsymbol{\varphi}_i}{\partial q_k} \dot{q}_k.$$

Then

$$\sum_{j=1}^{d} \dot{q}_j p_j - L(\mathbf{q}, \dot{\mathbf{q}}) = \frac{1}{2} \sum_{i=1}^{n} m_i \sum_{j,k=1}^{d} \frac{\partial \boldsymbol{\varphi}_i}{\partial q_j} \cdot \frac{\partial \boldsymbol{\varphi}_i}{\partial q_k} \dot{q}_j \dot{q}_k + \Phi(\mathbf{q}),$$

which is indeed the total mechanical energy.

Example: Consider the Harmonic oscillator whose Lagrangian is

$$L(q, \dot{q}) = \frac{m}{2}\dot{q}^2 - \frac{k}{2}q^2.$$

The momentum is $p = m\dot{q}$, so that we can easily express $\dot{q}$ as function of p. The Hamiltonian is

$$H(q, p) = \frac{p^2}{2m} + \frac{kq^2}{2}.$$

Hamilton's equations of motion are

$$\frac{dq}{dt} = \frac{p}{m} \qquad \frac{dp}{dt} = -kq.$$

Note that this system is not simpler than the one derived from the Lagrangian formulation. One extra-fact we can deduce from the conservation of the Hamiltonian is that the motion in phase-space is restricted to an ellipse. ▲

✎ *Exercise 7.3* Reverse the derivation of Hamilton's equations. Start from a Hamiltonian $H(q, p, t)$ with $q(t)$, $p(t)$ satisfying Hamilton's equations, and derive equations that treat q and $\dot{q}$ as independent variables through the Legendre transform of H with respect to the variable p.

✎ *Exercise 7.4* Suppose a system has a Lagrangian

$$L(q_1, q_2, \dot{q}_1, \dot{q}_2) = \dot{q}_1^2 + \frac{\dot{q}_2^2}{a + bq_1^2} + k_1 q_1^2 + k_2 \dot{q}_1 \dot{q}_2.$$

Find the equations of motion using the Hamiltonian formulation.

7.3 Symmetries and conservation laws

Recall that a generalized coordinate q_i is called cyclic if it does not appear explicitly in the Lagrangian. By the Lagrange equations of motion, the momentum p_i conjugate to q_i is conserved. Thus, if $p_i(0) = \alpha_i$ then $p_i(t) = \alpha_i$ for all t. Specifically, suppose that

$$L = L(q_2, \ldots, q_n, \dot{q}_1, \ldots, \dot{q}_n, t),$$

with $p_1(0) = \alpha_1$. Then, the Lagrange equations reduce to

$$\begin{aligned} &\frac{\partial L}{\partial \dot{q}_1}(q_2, \ldots, q_n, \dot{q}_1, \ldots, \dot{q}_n, t) = \alpha_1 \\ &\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}_i}\right) - \frac{\partial L}{\partial q_i} = 0 \qquad i = 2, \ldots, n. \end{aligned}$$

That is, the n differential equations are replaced by $n - 1$ differential equations supplemented by an algebraic equation. The presence of a cyclic coordinate does not allow the total elimination of the variables $q_1, \dot{q}_1$.

In the Hamiltonian formulation, a cyclic coordinate can be totally eliminated. First, we claim that if L does not depend on q_1, so does H. This is clear from the way H is constructed. Then, given that

$$H = H(q_2, \ldots, q_n, p_1, \ldots, p_n, t),$$

Hamilton's equations reduce to

$$\begin{aligned} \frac{dq_i}{dt} &= \frac{\partial H}{\partial p_i}(q_2, \ldots, q_n, \alpha_1, p_2, \ldots, p_n, t) \\ \frac{dp_i}{dt} &= -\frac{\partial H}{\partial q_i}(q_2, \ldots, q_n, \alpha_1, p_2, \ldots, p_n, t), \qquad i = 2, \ldots, n, \end{aligned}$$

i.e., (q_1, p_1) only affect the $n - 1$ equations through the value of conserved momentum. There is a real dimension reduction.

Thus, it is of practical importance to choose degrees of freedom in a way that makes as many cyclic coordinates as possible. The way to identify cyclic coordinate is through symmetries under which the dynamics ought to be invariant. For example, if the entire system is translationally invariance along a certain direction, a coordinate that represents the rigid motion of the system along this direction will be cyclic. Similar considerations apply for rigid rotations.

7.4 Derivation through a variational principle

Hamilton's equations can also be derived from a variational principle. The main difference with the Lagrangian representation is that $\mathbf{q}$ and $\mathbf{p}$ are viewed as independent coordinates. Thus, the functional to be minimized along the trajectory depends on two functions, $\mathbf{q}(t)$ and $\mathbf{p}(t)$. It is easy to guess what is the functional: it is still the action, which now takes the form,

$$I[\mathbf{q},\mathbf{p}] = \int_{t_1}^{t_2} \underbrace{\left(\sum_{i=1}^{n} p_i(t)\dot{q}_i(t) - H(\mathbf{q}(t),\mathbf{p}(t),t)\right)}_{f(\mathbf{q},\dot{\mathbf{q}},\mathbf{p},t)} dt.$$

The notable difference between the dependence of $\mathbf{q}$ and $\mathbf{p}$ is the dependence on $\dot{\mathbf{q}}$ but not $\dot{\mathbf{p}}$. Thus, we could require I to be extremal with respect to variations that keep $\mathbf{q}$ fixed at the end points, but imposing no restrictions on $\mathbf{p}$ at the end points. Then, the requirement $\delta I[\mathbf{q},\mathbf{p}] = 0$ results in

$$\frac{d}{dt}\left(\frac{\partial f}{\partial \dot{q}_i}\right) - \frac{\partial f}{\partial q_i} = 0 \quad \Rightarrow \quad \frac{dp_i}{dt} + \frac{\partial H}{\partial q_i} = 0,$$

and

$$\frac{\partial f}{\partial p_i} = 0 \quad \Rightarrow \quad \dot{q}_i - \frac{\partial H}{\partial p_i} = 0,$$

which are exactly Hamilton's equation. Yet, nothing prevents us from requiring that I be extremal with respect to paths that do not change $\mathbf{p}$ at the end points as well. There is nothing wrong in different variational principles to lead to the same equations. This additional restriction has advantages, for it allows us to even further modify the functional I. For example, we can freely add to $f(\mathbf{q},\dot{\mathbf{q}},\mathbf{p},t)$ a total time-derivative, since its integral depends only on the end point, hence it is not affected by variations. For example, we could subtract

$$\frac{d}{dt}\sum_{i=1}^{n} p_i q_i,$$

in which case the new functional is

$$\tilde{I}[\mathbf{q},\mathbf{p}] = \int_{t_1}^{t_2} \left(-\sum_{i=1}^{n} \dot{p}_i(t)q_i(t) - H(\mathbf{q}(t),\mathbf{p}(t),t)\right) dt.$$

It is easily checked that the resulting equations of motion are the same as before.

7.5 Final comments

Hamilton's equations of motion bring $\mathbf{q}$ and $\mathbf{p}$ to an equal level. Yet, the equations are only almost symmetric with respect to coordinates and momenta. There have been many attempts to obtain a totally symmetric formulation, but none of them provided any additional insight. There exists one such formulation which is of certain importance. The idea is to view $(\mathbf{q}, \mathbf{p})$ as one long vector $\boldsymbol{\eta}$ of size $2n$, with

$$\eta_i = q_i \qquad \eta_{i+n} = p_i.$$

Then, we view the Hamiltonian as a function $H(\boldsymbol{\eta})$. Its gradient is a $2n$ column vector with entries

$$\left(\frac{\partial H}{\partial \boldsymbol{\eta}}\right)_i = \frac{\partial H}{\partial q_i} \qquad \left(\frac{\partial H}{\partial \boldsymbol{\eta}}\right)_{i+n} = \frac{\partial H}{\partial p_i}.$$

We then introduce the $2n$-by-$2n$ anti-symmetric matrix J with entries

$$J = \begin{pmatrix} 0 & I_n \\ -I_n & 0 \end{pmatrix}.$$

Then, Hamilton's equations take the compact vector form

$$\frac{d\boldsymbol{\eta}}{dt} = J\frac{\partial H}{\partial \boldsymbol{\eta}}. \tag{7.5}$$

It may be easily verified that the matrix J satisfies the following algebraic properties,

$$J^2 = -I_{2n} \quad J^T = -J = J^{-1}, \qquad \text{and} \qquad \det J = 1.$$

The representation (7.5) is called the ***symplectic representation*** of Hamilton's equations.

Chapter 8

Canonical transformations

8.1 Motivation

Consider momentarily the case where all the coordinates $\mathbf{q}$ are cyclic. Then, all the corresponding momenta are conserved, $\mathbf{p} = \boldsymbol{\alpha}$, and Hamilton's equations reduce to

$$\frac{dq_i}{dt} = \frac{\partial H}{\partial p_i}(\boldsymbol{\alpha}) \equiv \omega_i,$$

with the trivial solution

$$q_i(t) = q_i(0) + \omega_i t.$$

Obviously, this is never then case, but one may ask whether by an ingenious change of variables it wouldn't be possible to obtain a new Hamiltonian system in which all the coordinates are cyclic.

This brings us to the following question: what type of (possibly time-dependent) transformations $(\mathbf{q}, \mathbf{p}) \to (\mathbf{Q}, \mathbf{P})$ retain the Hamiltonian structure. That is, there exists a function $K(\mathbf{Q}, \mathbf{P}, t)$ such that Hamilton's equations for $(\mathbf{q}, \mathbf{p})$ imply

$$\frac{dQ_i}{dt} = \frac{\partial K}{\partial P_i}$$
$$\frac{dP_i}{dt} = -\frac{\partial K}{\partial Q_i}.$$

Transformations that preserve the Hamiltonian structure of conjugate pairs of variables are call ***canonical transformations***.

8.2 Canonical transformations

Thus, we consider a change of variables,

$$Q_i = Q_i(\mathbf{q}, \mathbf{p}, t) \qquad \text{and} \qquad P_i = P_i(\mathbf{q}, \mathbf{p}, t).$$

This change of variables is assumed to be invertible, i.e., there exists an inverse transformation

$$q_i = q_i(\mathbf{Q}, \mathbf{P}, t) \qquad \text{and} \qquad p_i = p_i(\mathbf{Q}, \mathbf{P}, t).$$

We know that the time evolution of $(\mathbf{q}(t), \mathbf{p}(t))$ is governed by a variational principle, $\delta I[\mathbf{q}, \mathbf{p}] = 0$, with

$$I[\mathbf{q}, \mathbf{p}] = \int_{t_1}^{t_2} \left(\sum_{i=1}^{n} p_i \dot{q}_i - H(\mathbf{q}, \mathbf{p}, t) \right) dt.$$

The new variables $(\mathbf{Q}, \mathbf{P})$ would satisfy Hamilton's equations with a function K if their trajectory satisfies $\delta \tilde{I}[\mathbf{Q}, \mathbf{P}] = 0$, with

$$\tilde{I}[\mathbf{Q}, \mathbf{P}] = \int_{t_1}^{t_2} \left(\sum_{i=1}^{n} P_i \dot{Q}_i - K(\mathbf{Q}, \mathbf{P}, t) \right) dt.$$

We need to be precise: we can always require $\delta \tilde{I}[\mathbf{Q}, \mathbf{P}] = 0$ yielding Hamilton's equations for the new variables, but there is no guarantee that the resulting equations are compatible with Hamilton's equations for $(\mathbf{q}, \mathbf{p})$. What is needed, is that $\tilde{I}$ be extremal for the same trajectory that makes I extremal. This would happen, for example, if the integrands were identical. But recall that we have an additional freedom: we are free to modify the integrand by a total time derivative without affecting the variational problem. Thus, $(\mathbf{Q}, \mathbf{P})$ satisfy Hamilton's equations with function K if (but not only if!)

$$\sum_{i=1}^{n} p_i \dot{q}_i - H(\mathbf{q}, \mathbf{p}, t) = \sum_{i=1}^{n} P_i \dot{Q}_i - K(\mathbf{Q}, \mathbf{P}, t) + \frac{dF}{dt}. \tag{8.1}$$

The function F is called the ***generating function*** of the canonical transformation. The identity (8.1) has to hold for every choice of $\mathbf{q}(t)$, $\mathbf{p}(t)$, and this determines the relation between $(\mathbf{q}, \mathbf{p}, t)$ and $(\mathbf{Q}, \mathbf{P}, t)$.

We are now going to see a number of classes of generating functions F and the resulting canonical transformations.

8.3 Choices of generating functions

Suppose first that we take a generating function of the form

$$F = F_1(\mathbf{q}, \mathbf{Q}, t).$$

Substituting into (8.1) we get

$$\sum_{i=1}^{n}\left(p_i - \frac{\partial F_1}{\partial q_i}\right)\dot{q}_i - \left(H - K + \frac{\partial F_1}{\partial t}\right) - \sum_{i=1}^{n}\left(P_i + \frac{\partial F_1}{\partial Q_i}\right)\dot{Q}_i = 0.$$

It is important to realize that this identity has to hold no matter how we evolve $\mathbf{q}(t)$ and $\mathbf{p}(t)$ (hence $\mathbf{Q}(t)$ and $\mathbf{P}(t)$) in time. Therefore, we must have

$$\begin{aligned} p_i &= \frac{\partial F_1}{\partial q_i} \\ P_i &= -\frac{\partial F_1}{\partial Q_i} \\ K &= H + \frac{\partial F_1}{\partial t}. \end{aligned}$$

The first two sets of n equations determine the relation $(\mathbf{q}, \mathbf{p}, t) \mapsto (\mathbf{Q}, \mathbf{P}, t)$.

Example: As a simple (though trivial) example, consider the choice of

$$F_1(\mathbf{q}, \mathbf{Q}, t) = \sum_{i=1}^{n} q_i Q_i,$$

in which case we obtain

$$p_i = Q_i \quad \text{and} \quad P_i = -q_i.$$

That is, this generating function generated a canonical transformation that has for only effect to interchange the roles of $\mathbf{p}$ and $\mathbf{q}$. The corresponding Hamiltonian is then

$$K(\mathbf{Q}, \mathbf{P}) = H(-\mathbf{P}, \mathbf{Q}).$$

▲

The next set of generating functions is of the form

$$F = -\sum_{i=1}^{n} P_i Q_i + F_2(\mathbf{q}, \mathbf{P}, t).$$

Substituting into (8.1) we get

$$\sum_{i=1}^{n}\left(p_i - \frac{\partial F_2}{\partial q_i}\right)\dot{q}_i - \left(H - K + \frac{\partial F_2}{\partial t}\right) + \sum_{i=1}^{n}\left(Q_i - \frac{\partial F_2}{\partial P_i}\right)\dot{P}_i = 0.$$

By the same argument as before this implies

$$\begin{aligned} p_i &= \frac{\partial F_2}{\partial q_i} \\ Q_i &= \frac{\partial F_2}{\partial P_i} \\ K &= H + \frac{\partial F_2}{\partial t}. \end{aligned}$$

Example: If we take

$$F_2(\mathbf{q}, \mathbf{P}, t) = \sum_{i=1}^{n} q_i P_i,$$

then we get

$$p_i = P_i \quad \text{and} \quad Q_i = q_i,$$

i.e., the identity transformation. ▲

Example: Consider the case where

$$F_2(\mathbf{q}, \mathbf{P}, t) = \sum_{i=1}^{n} f_i(\mathbf{q}) P_i,$$

for some i. Then,

$$p_i = \sum_{j=1}^{n} \frac{\partial f_j}{\partial q_i} P_j \quad \text{and} \quad Q_i = f_i(\mathbf{q}).$$

If the Jacobian matrix with entries $\partial f_j / \partial q_i$ is invertible then $\mathbf{P}$ can be extracted. Thus we obtain that every ***invertible point transformation*** generates a canonical transformation. ▲

Next, consider generating functions of the form

$$F = \sum_{i=1}^{n} q_i p_i + F_3(\mathbf{p}, \mathbf{Q}, t).$$

Substituting into (8.1) we get

$$\sum_{i=1}^{n}\left(q_i - \frac{\partial F_3}{\partial p_i}\right)\dot{p}_i - \left(H - K + \frac{\partial F_3}{\partial t}\right) - \sum_{i=1}^{n}\left(P_i + \frac{\partial F_3}{\partial Q_i}\right)\dot{Q}_i = 0.$$

We then get

$$\begin{aligned} q_i &= \frac{\partial F_3}{\partial p_i} \\ P_i &= -\frac{\partial F_3}{\partial Q_i} \\ K &= H + \frac{\partial F_3}{\partial t}. \end{aligned}$$

✎ *Exercise 8.1* Work out the case where

$$F = \sum_{i=1}^{n} q_i p_i - \sum_{i=1}^{n} Q_i P_i + F_4(\mathbf{p}, \mathbf{P}, t).$$

Example: As a final example that shows how to kill a fly with a hammer, consider the harmonic oscillator, whose Hamiltonian is

$$H(q,p) = \frac{p^2}{2m} + \frac{kq^2}{2} = \frac{p^2}{2m} + \frac{m\omega^2 q^2}{2},$$

where $\omega^2 = k/m$. Consider now the canonical transformation with generating function

$$F_1(q,Q) = \frac{m\omega q^2}{2}\cot Q.$$

Then,

$$p = m\omega q\,\cot Q \quad \text{and} \quad P = \frac{m\omega q^2}{2}\sin^{-2} Q.$$

Also,

$$K(Q,P) = H(q(Q,P), p(Q,P)).$$

Substituting

$$q^2 = \frac{2P}{m\omega}\sin^2 Q \quad \text{and} \quad p^2 = 2Pm\omega\cos^2 Q,$$

we obtain

$$K(Q,P) = P\omega\cos^2 Q + P\omega\sin^2 Q = \omega P.$$

Since the (Q, P) is Hamiltonian (that's the whole point about canonical transformations!), the equations of motion are

$$\dot{Q} = \omega \quad \text{and} \quad \dot{P} = 0,$$

with the trivial solution,

$$P(t) = P(0) \quad \text{and} \quad Q(t) = Q(0) + \omega t.$$

Reverting back to the (q, p) variables we find

$$\begin{aligned} q(t) &= \sqrt{\frac{2P(0)}{m\omega}} \sin(Q(0) + \omega t) \\ p(t) &= \sqrt{2P(0)m\omega} \cos(Q(0) + \omega t). \end{aligned}$$

This is indeed the solution of the harmonic oscillator. As a last twist, note that $P(0) = K(Q(0), P(0))/\omega$, i.e., $P(0) = E/\omega$, and we can write

$$\begin{aligned} q(t) &= \sqrt{\frac{2E}{m\omega^2}} \sin(Q(0) + \omega t) \\ p(t) &= \sqrt{2Em} \cos(Q(0) + \omega t). \end{aligned}$$

▲

It is important to stress that every generating function F of the above form corresponds to a canonical transformation. The opposite is not true—not every canonical transformation corresponds to one of those four classes.

8.4 The symplectic approach

Another way to derive canonical transformations is the following. For simplicity, let's assume that the transformation is not time-dependent, i.e.,

$$\mathbf{Q} = \mathbf{Q}(\mathbf{q}, \mathbf{p}) \qquad \text{and} \qquad \mathbf{P} = \mathbf{P}(\mathbf{q}, \mathbf{p}).$$

In this case, we expect the Hamiltonian not to change.

Given that $(\mathbf{q}, \mathbf{p})$ are canonical pairs, the evolution of $(\mathbf{Q}, \mathbf{P})$ is derived from the chain rule,

$$\begin{aligned} \dot{Q}_i &= \sum_{j=1}^{n} \left(\frac{\partial Q_i}{\partial q_j} \dot{q}_j + \frac{\partial Q_i}{\partial p_j} \dot{p}_j \right) = \sum_{j=1}^{n} \left(\frac{\partial Q_i}{\partial q_j} \frac{\partial H}{\partial p_j} - \frac{\partial Q_i}{\partial p_j} \frac{\partial H}{\partial q_j} \right) \\ \dot{P}_i &= \sum_{j=1}^{n} \left(\frac{\partial P_i}{\partial q_j} \dot{q}_j + \frac{\partial P_i}{\partial p_j} \dot{p}_j \right) = \sum_{j=1}^{n} \left(\frac{\partial P_i}{\partial q_j} \frac{\partial H}{\partial p_j} - \frac{\partial P_i}{\partial p_j} \frac{\partial H}{\partial q_j} \right). \end{aligned}$$

On the other hand, we wish to have

$$\dot{Q}_i = \frac{\partial H}{\partial P_i} = \sum_{j=1}^{n} \left(\frac{\partial H}{\partial q_j} \frac{\partial q_j}{\partial P_i} + \frac{\partial H}{\partial p_j} \frac{\partial p_j}{\partial P_i} \right)$$

$$\dot{P}_i = -\frac{\partial H}{\partial Q_i} = -\sum_{j=1}^{n} \left(\frac{\partial H}{\partial q_j} \frac{\partial q_j}{\partial Q_i} + \frac{\partial H}{\partial p_j} \frac{\partial p_j}{\partial Q_i} \right).$$

These two sets of equations can be written is matrix form

$$\frac{d}{dt} \begin{pmatrix} \mathbf{Q} \\ \mathbf{P} \end{pmatrix} = \begin{pmatrix} -D_{\mathbf{p}}\mathbf{Q} & D_{\mathbf{q}}\mathbf{Q} \\ -D_{\mathbf{p}}\mathbf{P} & D_{\mathbf{q}}\mathbf{P} \end{pmatrix} \begin{pmatrix} D_{\mathbf{q}}H \\ D_{\mathbf{p}}H \end{pmatrix},$$

and

$$\frac{d}{dt} \begin{pmatrix} \mathbf{Q} \\ \mathbf{P} \end{pmatrix} = \begin{pmatrix} D_{\mathbf{P}}\mathbf{q} & -D_{\mathbf{Q}}\mathbf{q} \\ D_{\mathbf{P}}\mathbf{p} & -D_{\mathbf{Q}}\mathbf{p} \end{pmatrix}^T \begin{pmatrix} D_{\mathbf{q}}H \\ D_{\mathbf{p}}H \end{pmatrix}.$$

Since the identity between the right-hand sides must hold for all systems, it must be that

$$-(D_{\mathbf{p}}\mathbf{Q})_{ij} = (D_{\mathbf{P}}\mathbf{q})^T_{ij} \quad \Rightarrow \quad -\frac{\partial Q_i}{\partial p_j} = \frac{\partial q_j}{\partial P_i}$$

$$(D_{\mathbf{q}}\mathbf{Q})_{ij} = (D_{\mathbf{P}}\mathbf{p})^T_{ij} \quad \Rightarrow \quad \frac{\partial Q_i}{\partial q_j} = \frac{\partial p_j}{\partial P_i}$$

$$(D_{\mathbf{p}}\mathbf{P})_{ij} = (D_{\mathbf{Q}}\mathbf{q})^T_{ij} \quad \Rightarrow \quad \frac{\partial P_i}{\partial p_j} = \frac{\partial q_j}{\partial Q_i}$$

$$(D_{\mathbf{q}}\mathbf{P})_{ij} = -(D_{\mathbf{Q}}\mathbf{p})^T_{ij} \quad \Rightarrow \quad \frac{\partial P_i}{\partial q_j} = -\frac{\partial p_j}{\partial Q_i}$$

Recall that these are functional relations (no dynamics). If they hold, then the transformation is canonical with the same Hamiltonian (expressed as a function of the new variables).

✎ *Exercise 8.2* Show that the transformation

$$Q = \log\left(\frac{1}{q}\sin p\right) \qquad P = q\,\cot p$$

is canonical.

✎ *Exercise 8.3* Consider the following transformation,

$$Q = \log\left(1 + \sqrt{q}\,\cos p\right) \qquad P = 2(1 + \sqrt{q}\,\cos p)\,\sqrt{q}\,\sin p.$$

(i) Show that it is canonical. (ii) Show that is can be derived using the generating function $F_3(Q,p) - (e^Q - 1)^2 \tan p$.

✎ *Exercise 8.4* Show that canonical transformations form a group.

We can repeat the above characterization using the symplectic representation. Recall that Hamilton's equations read

$$\frac{d\boldsymbol{\eta}}{dt} = J\frac{\partial H}{\partial \boldsymbol{\eta}}.$$

Consider now a change of variables $\boldsymbol{\eta} \mapsto \boldsymbol{\xi}(\boldsymbol{\eta})$. Then,

$$\frac{d\boldsymbol{\xi}}{dt} = (D_{\boldsymbol{\eta}}\boldsymbol{\xi})\frac{d\boldsymbol{\eta}}{dt} = (D_{\boldsymbol{\eta}}\boldsymbol{\xi})J\frac{\partial H}{\partial \boldsymbol{\eta}} = (D_{\boldsymbol{\eta}}\boldsymbol{\xi})J(D_{\boldsymbol{\eta}}\boldsymbol{\xi})^T\frac{\partial H}{\partial \boldsymbol{\xi}}.$$

Thus, the transformation is canonical if

$$J = (D_{\boldsymbol{\eta}}\boldsymbol{\xi})J(D_{\boldsymbol{\eta}}\boldsymbol{\xi})^T \qquad \text{or} \qquad J_{ij} = \sum_{k,\ell=1}^{2n} \frac{\partial \xi_i}{\partial \eta_k} J_{k\ell} \frac{\partial \xi_j}{\partial \eta_\ell}.$$

Finally, we claim that this symplectic condition remains valid also in the time-dependent case. It require tedious though straightforward algebra to show it.

8.5 Poisson brackets

Definition 8.1 *Let* $(\mathbf{q},\mathbf{p})$ *be canonical variables and* $u = u(\mathbf{q},\mathbf{p})$, $v = v(\mathbf{q},\mathbf{p})$. *We define*

$$\{u,v\}_{\mathbf{q},\mathbf{p}} = \sum_{i=1}^{n}\left(\frac{\partial u}{\partial q_i}\frac{\partial v}{\partial p_i} - \frac{\partial u}{\partial p_i}\frac{\partial v}{\partial q_i}\right).$$

The Poisson brackets map two functions into a new function. It is a bi-linear anti-symmetric product. In symplectic form it becomes

$$\{u,v\}_{\boldsymbol{\eta}} = (D_{\boldsymbol{\eta}}u)^T J(D_{\boldsymbol{\eta}}v) = \sum_{i,j=1}^{2n} \frac{\partial u}{\partial \eta_i} J_{ij} \frac{\partial v}{\partial \eta_j}.$$

In particular we note that

$$\left\{q_i, q_j\right\}_{\mathbf{q},\mathbf{p}} = \left\{p_i, p_j\right\}_{\mathbf{q},\mathbf{p}} = 0 \qquad \text{and} \qquad \left\{q_i, p_j\right\}_{\mathbf{q},\mathbf{p}} = \delta_{ij}.$$

In symplectic notation

$$\left\{\eta_i, \eta_j\right\}_{\boldsymbol{\eta}} = J_{ij}.$$

Let u, v be two functions of $(\mathbf{q}, \mathbf{p})$ and consider a canonical transformation $(\mathbf{q}, \mathbf{p}) \mapsto (\mathbf{Q}, \mathbf{P})$. How do Poisson brackets transform, i.e., what is the relation between

$$\{u, v\}_{\mathbf{q},\mathbf{p}} \qquad \text{and} \qquad \{u, v\}_{\mathbf{Q},\mathbf{P}}?$$

It is more convenient to do it in the symplectic notation, although you can easily verify it within the $(\mathbf{q}, \mathbf{p})$ notation. Thus, for a canonical transformation $\boldsymbol{\xi}(\boldsymbol{\eta})$,

$$\{u, v\}_{\boldsymbol{\xi}} = (D_{\boldsymbol{\xi}} u)^T J (D_{\boldsymbol{\xi}} v) = (D_{\boldsymbol{\eta}} u)^T (D_{\boldsymbol{\xi}} \boldsymbol{\eta})^T J (D_{\boldsymbol{\xi}} \boldsymbol{\eta})(D_{\boldsymbol{\eta}} v).$$

Noting that $(D_{\boldsymbol{\xi}} \boldsymbol{\eta}) = (D_{\boldsymbol{\eta}} \boldsymbol{\xi})^{-1}$, the center part is found to be equal to J (the symplectic condition), and we end up with

$$\{u, v\}_{\boldsymbol{\xi}} = \{u, v\}_{\boldsymbol{\eta}},$$

i.e., *Poisson brackets are invariant under canonical transformations*.

Recall that Hamilton's equations have the property of remaining invariant under canonical transformations. Similarly, equations expressed in terms of Poisson brackets will be invariant under such transformations. It is indeed possible to reformulation classical mechanics completely in terms of Poisson brackets. The remarkable fact is that this reformulations can be extended with little change into the laws of quantum mechanics.

The Poisson bracket can be viewed as a product operation between functions of phase-space (and possibly time). This product together with the vector field character of functions produces an ***algebra***. The algebraic properties of the Poisson bracket are:

1. Anti-symmetry.

2. Bilinearity.

3. $\{uv, w\} = u\{v, w\} + \{u, w\} v$ (follows from the laws of differentiation).

4. Jacobi's identity, $\{u, \{v, w\}\} + \{w, \{u, v\}\} + \{v, \{w, u\}\} = 0$.

The proof of Jacobi's identity is somewhat lengthy and only technical. Note that

$$\{u,\{v,w\}\} = \frac{\partial u}{\partial \eta_i} J_{ij} \frac{\partial}{\partial \eta_j}\left(\frac{\partial v}{\partial \eta_k} J_{k\ell} \frac{\partial w}{\partial \eta_\ell}\right) = \frac{\partial u}{\partial \eta_i} J_{ij} J_{k\ell}\left(\frac{\partial^2 v}{\partial \eta_j \partial \eta_k}\frac{\partial w}{\partial \eta_\ell} + \frac{\partial v}{\partial \eta_k}\frac{\partial^2 w}{\partial \eta_j \partial \eta_\ell}\right)$$

(with summation over repeated indexes). To this we need to add the cyclic permutations,

$$\{v,\{w,u\}\} = \frac{\partial v}{\partial \eta_i} J_{ij} J_{k\ell}\left(\frac{\partial^2 w}{\partial \eta_j \partial \eta_k}\frac{\partial u}{\partial \eta_\ell} + \frac{\partial w}{\partial \eta_k}\frac{\partial^2 u}{\partial \eta_j \partial \eta_\ell}\right)$$

$$\{w,\{u,v\}\} = \frac{\partial w}{\partial \eta_i} J_{ij} J_{k\ell}\left(\frac{\partial^2 u}{\partial \eta_j \partial \eta_k}\frac{\partial v}{\partial \eta_\ell} + \frac{\partial u}{\partial \eta_k}\frac{\partial^2 v}{\partial \eta_j \partial \eta_\ell}\right).$$

Consider, for example, all the terms where w is differentiated twice:

$$\frac{\partial u}{\partial \eta_i} J_{ij} J_{k\ell} \frac{\partial v}{\partial \eta_k}\frac{\partial^2 w}{\partial \eta_j \partial \eta_\ell} + \frac{\partial v}{\partial \eta_i} J_{ij} J_{k\ell} \frac{\partial^2 w}{\partial \eta_j \partial \eta_k}\frac{\partial u}{\partial \eta_\ell}.$$

Since the indexes are all dummy indexes, we may rename them in the second term, $i \to k$, $\ell \to i$, $k \to j$, and $j \to \ell$

$$\frac{\partial u}{\partial \eta_i} J_{ij} J_{k\ell} \frac{\partial v}{\partial \eta_k}\frac{\partial^2 w}{\partial \eta_j \partial \eta_\ell} + \frac{\partial v}{\partial \eta_k} J_{k\ell} J_{ji} \frac{\partial^2 w}{\partial \eta_\ell \partial \eta_j}\frac{\partial u}{\partial \eta_i} = 0,$$

where we have used the anti-symmetry of J.

The Poisson bracket algebra is non-associative. Jacobi's identity replaces in fact the law of associativity. An algebra satisfying these properties is known as a ***Lie algebra***.

Comment: Other Lie algebras are the vector product of vectors, $(\boldsymbol{a},\boldsymbol{b}) \mapsto \boldsymbol{a}\times\boldsymbol{b}$ and the commutator of square matrices, $(A,B) = AB - BA$.

We end this section be noting another very important canonical invariant. Recall that a canonical transformation $\boldsymbol{\xi}(\boldsymbol{\eta})$ satisfies,

$$J = (D_{\boldsymbol{\eta}}\boldsymbol{\xi}) J (D_{\boldsymbol{\eta}}\boldsymbol{\xi})^T.$$

Hence,

$$\det J = \det(D_{\boldsymbol{\eta}}\boldsymbol{\xi}) \cdot \det J \cdot \det(D_{\boldsymbol{\eta}}\boldsymbol{\xi}),$$

and

$$|\det(D_{\boldsymbol{\eta}}\boldsymbol{\xi})| = 1.$$

This means that canonical transformation conserve phase-space volume!

8.6 Poisson bracket formulation of mechanics

Consider any differentiable function $u(\mathbf{q}, \mathbf{p}, t)$. Its time derivative along a Hamiltonian trajectory is

$$\frac{d}{dt}u(\mathbf{q}(t), \mathbf{p}(t), t) = \sum_{i=1}^{n}\left(\frac{\partial u}{\partial q_i}\frac{dq_i}{dt} + \frac{\partial u}{\partial p_i}\frac{dp_i}{dt}\right) + \frac{\partial u}{\partial t} = \{u, H\}_{\mathbf{q},\mathbf{p}} + \frac{\partial u}{\partial t}.$$

This equation, which governs the dynamics of any ***observable*** under Hamiltonian dynamics encompasses the laws of mechanics. In particular,

$$\frac{d\boldsymbol{\eta}}{dt} = \{\boldsymbol{\eta}, H\}_{\eta}.$$

Note that an immediate consequence is

$$\frac{dH}{dt} = \frac{\partial H}{\partial t},$$

i.e., the conservation of the Hamiltonian when it is not explicitly time-dependent. Moreover, any function $u(\mathbf{q}, \mathbf{p}, t)$ is a constant of motion if and only if,

$$\{u, H\}_{\mathbf{q},\mathbf{p}} + \frac{\partial u}{\partial t} = 0.$$

Moreover, it follows that if both u, v are constants of motion so is $\{u, v\}$. Indeed, by Jacobi's identity and the anti-symmetry of the Poisson bracket,

$$\{H, (u, v)\} = -\{u, (v, H)\} - \{v, (H, u)\} = \left\{u, \frac{\partial v}{\partial t}\right\} - \left\{v, \frac{\partial u}{\partial t}\right\} = \frac{\partial}{\partial t}\{u, v\}.$$

This may give a way to generate many invariants of motion. In most cases, however, this process terminates fast, yielding trivial variables. A class of systems for which infinitely many conserved quantities can be thus generated are ***integrable systems*** (if you ever encounter the theory of ***solitons***).

8.7 Differentiable transformations

So far, we discussed canonical transformations $\boldsymbol{\eta} \mapsto \boldsymbol{\xi}$. We now extend the treatment to a continuous family of such transformations, depending on a continuous parameter s, i.e.,

$$\boldsymbol{\xi} = \boldsymbol{\xi}(\boldsymbol{\eta}, s),$$

where $\boldsymbol{\xi}(\boldsymbol{\eta}, 0) = \boldsymbol{\eta}$. That is, we start with a set of canonical variables $\boldsymbol{\eta}$ and continuous transition to new sets of canonical variables $\boldsymbol{\xi}$.

As we' have seen, for every s, we have

$$(D_{\boldsymbol{\eta}}\boldsymbol{\xi})J(D_{\boldsymbol{\eta}}\boldsymbol{\xi})^T = J,$$

or component-wise,

$$\sum_{k,\ell=1}^{2n} \frac{\partial \xi_i}{\partial \eta_k} J_{k\ell} \frac{\partial \xi_j}{\partial \eta_\ell} = J_{ij}.$$

Differentiating with respect to s we get

$$\sum_{k,\ell=1}^{2n} \left(\frac{\partial \xi_i'}{\partial \eta_k} J_{k\ell} \frac{\partial \xi_j}{\partial \eta_\ell} + \frac{\partial \xi_i}{\partial \eta_k} J_{k\ell} \frac{\partial \xi_j'}{\partial \eta_\ell} \right) = 0, \tag{8.2}$$

where the prove denotes here the partial derivative with respect to s. This last equation characterizes a "dynamics" of canonical transformations. The derivative with respect the variable s describes an evolution along an axis of continuous change of variables.

Suppose now that we identify the parameter s with time, and let $\boldsymbol{\xi}(\boldsymbol{\eta}, t)$ evolve according to the Hamiltonian dynamics,

$$\xi_i'(\boldsymbol{\eta}, t) = \sum_{r=1}^{2n} J_{ir} \frac{\partial H}{\partial \eta_j}(\boldsymbol{\xi}(\boldsymbol{\eta}, t), t).$$

Then,

$$\frac{\partial \xi_i'}{\partial \eta_k} = \sum_{r,m=1}^{2n} J_{ir} \frac{\partial^2 H}{\partial \eta_r \partial \eta_m} \frac{\partial \xi_m}{\partial \eta_k}$$

and upon substituting into the left-hand side of (8.2) we get

$$\sum_{k,\ell,m,r=1}^{2n} \left(J_{ir} \frac{\partial^2 H}{\partial \eta_r \partial \eta_m} \frac{\partial \xi_m}{\partial \eta_k} J_{k\ell} \frac{\partial \xi_j}{\partial \eta_\ell} + \frac{\partial \xi_i}{\partial \eta_k} J_{k\ell} J_{jr} \frac{\partial^2 H}{\partial \eta_r \partial \eta_m} \frac{\partial \xi_m}{\partial \eta_\ell} \right).$$

We need to show that this is zero. Here is a not-too-formal argument: suppose that the transformation was canonical at time t. Then this expression equals

$$\sum_{r,m=1}^{2n} \left(J_{ir} \frac{\partial^2 H}{\partial \eta_r \partial \eta_m} J_{mj} + J_{im} J_{jr} \frac{\partial^2 H}{\partial \eta_r \partial \eta_m} \right).$$

Interchanging the indexes r and m, this expression vanishes by the anti-symmetry of J. Thus, if

$$(D_\eta \xi) J (D_\eta \xi)^T - J = 0$$

at time t then

$$\frac{d}{dt}\left[(D_\eta \xi) J (D_\eta \xi)^T - J\right] = 0.$$

Now to the formal argument: in matrix notation,

$$\frac{d}{dt}\left[(D_\eta \xi) J (D_\eta \xi)^T - J\right] = (D_\eta \xi') J (D_\eta \xi)^T + (D_\eta \xi) J (D_\eta \xi')^T,$$

and

$$(D_\eta \xi') = J(D^2 H)(D_\eta \xi),$$

hence

$$\frac{d}{dt}\left[(D_\eta \xi) J (D_\eta \xi)^T - J\right] = J(D^2 H)(D_\eta \xi) J (D_\eta \xi)^T - (D_\eta \xi) J (D_\eta \xi)^T (D^2 H) J.$$

subtracting from the right hand side

$$J(D^2 H) J - J(D^2 H) J = 0,$$

we get for $S = (D_\eta \xi) J (D_\eta \xi)^T - J$

$$\frac{dS}{dt} = J(D^2 H) S - S (D^2 H) J.$$

This is a linear equation for S, and $S = 0$ is a fixed point. Thus, $S(0) = 0$ implies $S(t) = 0$ for all times.

8.8 Liouville's theorem

Having seen that canonical transformations preserve the Lebesgue measure and that the Hamiltonian flow induces a differentiable family of canonical transformations, it follow at once that Hamiltonian dynamics are measure preserving. This property is known a ***Liouville's theorem***. To state it precisely, let $A \subset \mathbb{R}^{2n}$ be a finite volume in phase space. For each t the dynamics induce a transformation

$T_t(\mathbf{q}, \mathbf{p})$, which is the evolute of the mechanical system that has started as time zero from the point $(\mathbf{q}, \mathbf{p})$. Liouville's theorem states that

$$\mu(T_t(A)) = \mu(A).$$

The transformation T_t is a measure preserving mapping from the phase-space into itself. Mappings that have this property define a ***measure preserving dynamical system***, which constitute a classical field of mathematical research.

Chapter 9

The Hamilton-Jacobi theory

9.1 The Hamilton-Jacobi equation

Let $\mathbf{q}, \mathbf{p}$ be canonical variables. Their time evolution satisfies Hamilton's equations,

$$\frac{dq_i}{dt} = \frac{\partial H}{\partial p_i} \qquad \frac{dp_i}{dt} = -\frac{\partial H}{\partial q_i}.$$

Denote the initial data by $\mathbf{q}(0) = \mathbf{Q}$ and $\mathbf{p}(0) = \mathbf{P}$. Hamilton's equation induce a time-dependent mapping,

$$(\mathbf{Q}, \mathbf{P}) \mapsto (\mathbf{q}(t), \mathbf{p}(t)),$$

such that in fact, one should write

$$\mathbf{q} = \mathbf{q}(\mathbf{Q}, \mathbf{P}, t) \qquad \text{and} \qquad \mathbf{p} = \mathbf{p}(\mathbf{Q}, \mathbf{P}, t).$$

(The Hamiltonian dynamics define a ***flow*** in phase space.) We can also refer to the inverse mapping,

$$\mathbf{Q} = \mathbf{Q}(\mathbf{q}, \mathbf{p}, t) \qquad \text{and} \qquad \mathbf{P} = \mathbf{P}(\mathbf{q}, \mathbf{p}, t).$$

In the previous section, we saw that this mapping was in fact canonical. Finding this mapping mean solving the differential system: expressing the coordinates and momenta at time t given their values at time zero. The Hamilton-Jacobi theory aims precisely at finding this mapping.

How to proceed. Knowing that a mapping is canonical means that it has a certain structure that its Jacobian must satisfy. Moreover, the transformed variables satisfy Hamiltonian dynamics with a transformed Hamiltonian. In the present case, we want the new variables $(\mathbf{Q}, \mathbf{P})$ to be stationary in time, since we want

$$\mathbf{q}(t) = \mathbf{q}(\mathbf{Q}(t), \mathbf{P}(t), t) = \mathbf{q}(\mathbf{Q}(0), \mathbf{P}(0), t).$$

A way to impose it is to require the transformed Hamiltonian K to be, say, zero (could be any function of time only). Suppose furthermore that we try to generate this transformation using a generating function of the form $F_2(\mathbf{q}, \mathbf{P}, t)$ (here again, the choice of generating function is somewhat arbitrary). Then, as seen in the previous section,

$$K = H(\mathbf{q}, \mathbf{p}, t) + \frac{\partial F_2}{\partial t}(\mathbf{q}, \mathbf{P}, t) = 0,$$

and

$$p_i = \frac{\partial F_2}{\partial q_i} \qquad Q_i = \frac{\partial F_2}{\partial P_i}.$$

Using the first of the canonical relations, and substituting it into the Hamiltonian transformation, we obtain

$$\frac{\partial F_2}{\partial t}(\mathbf{q}, \mathbf{P}, t) + H\left(\mathbf{q}, \frac{\partial F_2}{\partial \mathbf{q}}(\mathbf{q}, \mathbf{P}, t), t\right) = 0. \tag{9.1}$$

This is the Hamilton-Jacobi equation. Fixing $\mathbf{P}$ (the initial data for the momentum) and defining

$$S(\mathbf{q}, t) = F_2(\mathbf{q}, \mathbf{P}, t),$$

equation (9.1) takes the form

$$\frac{\partial S}{\partial t} + H\left(\mathbf{q}, \frac{\partial S}{\partial \mathbf{q}}, t\right) = 0.$$

It is a first order ***partial differential equation*** in $(n + 1)$ variables. Its solution is a generating function (with $\mathbf{P}$ as a parameter), which we can use in order to find the mapping between the coordinates at time zero and time t.

Comment: A PDE in $n + 1$ variables is by no means simpler that a system of $2n$ ODEs. The transition from first-order PDEs and systems of ODEs is standard in the analysis of hyperbolic PDEs.

Suppose we solve the equation for S. Since it is a first-order equation in $n+1$ variables, the solution involves $n+1$ integration constant. Note however that S is only defined up to an additive constant, which will not affect the generating function anyways. Thus, without loss of generality, S depends on n integration constants $\boldsymbol{\alpha}$,

$$S = S(\mathbf{q}, \boldsymbol{\alpha}, t).$$

Since these constants are arbitrary, we are free to identify them with the momenta $\mathbf{P}$, i.e., set

$$F_2(\mathbf{q}, \mathbf{P}, t) = S(\mathbf{q}, \mathbf{P}, t).$$

(Note that the way of writing a solution with n integration constants is not unique, nut any form will do). Now we can proceed,

$$p_i = \frac{\partial S}{\partial q_i}(\mathbf{q}, \mathbf{P}, t) \qquad \text{and} \qquad Q_i = \frac{\partial S}{\partial P_i}(\mathbf{q}, \mathbf{P}, t).$$

Inverting these equations provides the desired solution.

9.2 An example

We have our beloved example—the Harmonic oscillator. Recall that

$$H(q, p) = \frac{1}{2m}(p^2 + m^2\omega^2 q^2).$$

The Hamilton-Jacobi equation for $S(q, t)$ is

$$\frac{\partial S}{\partial t} + \frac{1}{2m}\left[\left(\frac{\partial S}{\partial q}\right)^2 + m^2\omega^2 q^2\right] = 0.$$

Look then for a solution of the form

$$S(q, t) = A(q) - \alpha t.$$

Substituting we get

$$\alpha = \frac{1}{2m}\left[(A'(q))^2 + m^2\omega^2 q^2\right],$$

which is a first-order equation for $A(q)$. We at once get

$$A'(q) = \sqrt{2m\alpha}\sqrt{1 - \frac{m\omega^2}{2\alpha}q^2}.$$

I.e.,

$$S(q,t) = \int_0^q \sqrt{2m\alpha - m^2\omega^2 r^2}\, dr - \alpha t.$$

We can now identify the constant of integration α with the initial momentum P. The transformation equations are

$$p = \frac{\partial S}{\partial q} = \sqrt{2mP - m^2\omega^2 q^2}$$

and

$$Q = \frac{\partial S}{\partial P} = -t + m\int_0^q \frac{1}{\sqrt{2mP - m^2\omega^2 r^2}}\, dr.$$

The last integral can be easily solved,

$$Q = -t + \sqrt{\frac{m}{2P}}\int_0^q \frac{1}{\sqrt{1 - \frac{m\omega^2}{2P}r^2}}\, dr = -t + \frac{1}{\omega}\sin^{-1}\left(\sqrt{\frac{m\omega^2}{2P}}q\right).$$

This can easily be inverted,

$$q = \sqrt{\frac{2P}{m\omega^2}}\sin[\omega(t+Q)].$$

We can then extract p,

$$p = \sqrt{2mP}\cos[\omega(t+Q)].$$

Q, **P** CAN BE ANY PAIR OF VARIABLES THAT REFER TO TIME ZERO.

Chapter 10

Quantum mechanics

10.1 Matter and waves

Toward the end of the nineteenth century, there was a more or less unanimous feeling that the physical world has been fully elucidated, at least from a fundamental point of view. On the one hand, the was mechanics that provided a comprehensive description of material particles (in this respect, it does not matter which of the mechanical description is used since they are all equivalent). On the other hand, there was electromagnetism theory, which provided a full description of the laws of electricity, magnetism and light (hence optics). These two theories—that of particles and that of waves—were even related via the Lorentz law for the force that an electromagnetic field exerts on a charged particle. This utopic image was however shattered at the turn of the century, as a number of nagging experiments could not be interpreted by the existing physical theories. By two decades, the whole picture regarding the fundamental laws of nature was drastically changed.

The question whether light was made of particles or whether is was a wave (a propagating perturbation) was a matter of controversy for ages. Newton believed that light was made of tiny particles, but experiments revealed that light exhibits purely wave-like phenomena, such as interference and diffraction. Maxwell's equations of electromagnetism finally gave a coherent explanation for the nature of light, as an electromagnetic wave.

Let's concentrate on the two-slit experiment. A source of light emits light which is detected by a light detector that is behind an opaque wall with two narrow slits. Suppose that light was made of tiny particles that are emitted in all directions.

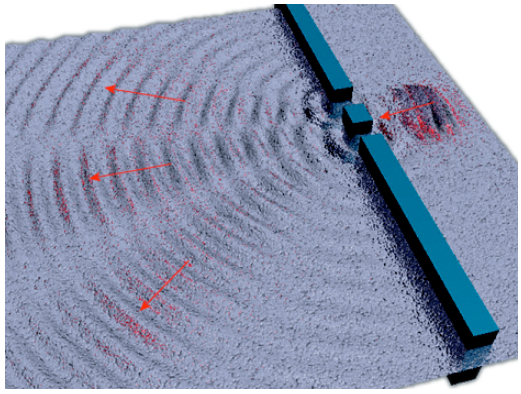


Figure 10.1: Visualization of a two-slit experiment

Then, some of those particle would get through the narrow slits and hit the detector behind. If this were the case, we would expect the detector to report a relatively high light intensity at two localized spots. Instead, one observes a striped pattern of light and darkness, with high intensity in locations that are not directly behind the slits. If, however, one of the lits is covered, then there is just one spot of high intensity behind the slit. This detected pattern is explained by the fact that light is a wave that satisfies a ***principle of superposition***. Every point on the detector receives electromagnetic waves coming from two sources (the slits); depending on the precise position on the detector, these two waves could interfer such to always cancel each other (a dark spot), or, on the contrary, they could interfer positively (a bright spot). Mathematically, an electromagnetic wave can be described by a complex vector-valued function of space and time $\boldsymbol{E}(\mathbf{r}, t)$. Two such waves have to be added,

$$\boldsymbol{E}(\mathbf{r}, t) = \boldsymbol{E}_1(\mathbf{r}, t) + \boldsymbol{E}_2(\mathbf{r}, t),$$

whereas the wave intensity is proportional to the modulus square of the electromagnetic field,

$$I(\mathbf{r}, t) = |\boldsymbol{E}(\mathbf{r}, t)|^2,$$

i.e., $I \neq I_1 + I_2$.

The vision of light as a wave was however shattered by the experiments of the ***photo-electric effect*** and its explanation by Einstein, which concluded that light was made of particles, ***photons***, whose energy was determined solely by their frequency (i.e., the color of light). For some time, there were attempts to explain the

wave-like nature of light as resulting from interactions between photons. However, it became possibly to perform the two-slit experiment by virtually releasing photons one-by-one, and still an interference patterns was obtained. Even though one believed that each photon has two pass through one of the two slits, it seemed as if it "knew" that it had another possibility and "interfered" with this other possibility. Any experiment that could determine through which slit the photon passed was found to "destroy" the experiment, i.e., destroy the interference pattern.

The real shock occurred when it was later found the electrons, clearly material entities, exhibit the exact same behavior in a two-slit experiment.

These and other findings led eventually to a new picture of matter and waves, whereby (1) material particles may exhibit both material-like and wave-like behavior, (2) this wave-like behavior is manifest in a superposition principle, (3) the behavior of the system is inherently ***random***, (4) experiment tend to drastically interfer with the state of the system.

It was Schrodinger who first proposed a description of the microscopic world along with dynamics. His view of a particle was that it is described by a complex-valued ***wave function***, $\psi(\mathbf{r}, t)$, with

$$\int_A |\psi(\mathbf{r}, t)|^2 \, d\mathbf{r}, \qquad A \subset \mathbb{R}^3,$$

being the probability of finding the particle in the set A at time t. If the particle has mass m and is in a potential field $V(\mathbf{r})$, then this wave function is governed by ***Schrodinger's equation***,

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \Delta\psi + V(\mathbf{r})\psi \equiv H\psi,$$

which is a partial differential equation. The quantity $\hbar$ is a physical constant, known as ***Planck's constant***.

Comment: Classical mechanics as an approximation to quantum mechanics and relativistic mechanics.

Another source of confusion was the discovery that light emitted from atoms always has frequencies of a restricted and discrete set of values (it has a fixed ***spectrum***). At that time, it was known that the emission of light is cause by a loss of energy of the electron that surround the atom. The implication was that electrons could only assume a discrete set of energies (the energies of the electrons were

said to be ***quantized***). While this situation was described by Niels Bohr in terms of ***energy shells***, the fact that the values of the energy could not assume any value could not be reconciled with classical mechanics.

10.2 The postulates of quantum mechanics

Quantum mechanics describes a physical system by a wave function. For a single particle, a wave function is a complex-valued function of space and time, $\psi(\mathbf{r}, t)$. Its modulus square is interpreted as the probability density to find the particle at time t in position $\mathbf{r}$. Since this density has to be normalized,

$$\int_{\mathbb{R}^3} |\psi(\mathbf{r}, t)|^2 \, d\mathbf{r} = 1,$$

it follows that ψ must be an element of the space of square-integrable functions, $L^2(\mathbb{R}^3)$. This is a Hilbert space, $\mathscr{H}$, when endowed with the inner product

$$(\phi, \psi) = \int_{\mathbb{R}^3} \phi^*(\mathbf{r})\psi(\mathbf{r}) \, d\mathbf{r}.$$

The inner-product is linear in its second argument and skew-linear in its first argument.

Measurable quantities (or ***observables***) are identified with linear operators on $\mathscr{H}$. A linear operator is a linear mapping $\mathscr{H} \to \mathscr{H}$. Every linear operator A has an adjoint A^* defined by

$$(\phi, A\psi) = (A^\dagger \phi, \psi).$$

An operator is called self-adjoint if $A = A^\dagger$ (also Hermitian).

With every linear operator is associated an eigenvalue problem,

$$Au = \lambda u.$$

A function u satisfying such a relation is called the eigenfunction corresponding to the eigenvalue λ. Self-adjoint operators have the property that all their eigenvalues are real and that their eigenfunction constitute an orthogonal basis in $\mathscr{H}$. The set of eigenvalues (the spectrum of A can be either discrete, continuous, or mixed). Continuous spectra are harder to deal with since the corresponding eigenfunction are not elements of $\mathscr{H}$ (they are distributions).

Let thus A be a self-adjoint operator with a discrete spectrum,

$$Au_k = \lambda_k u_k, \qquad k = 1, 2, \ldots.$$

Then, every wave function ψ has a unique decomposition,

$$\psi(\mathbf{r}) = \sum_{k=1}^{\infty} a_k u_k(\mathbf{r}).$$

Assuming that the u_k are normalized, it follows that

$$a_k = (u_k, \psi).$$

Parseval's identity, which we derive here without rigor, gives,

$$1 = (\psi, \psi) = \sum_{j,k=1}^{\infty} (a_k u_k, a_j u_j) = \sum_{k=1}^{\infty} |a_k|^2.$$

The postulates of quantum mechanics are the following:

① every measurable quantity is associated with a self-adjoint operator.

② The eigenvalues of this operator are the only possible outcomes of the measurement.

③ The outcome is random, and the probability of obtaining the value λ_k is $|a_k|^2$.

④ After the measurement has been done, the wave function becomes the eigenfunction u_k (the wave function is said to ***collapse*** according to the outcome of the measurement).

⑤ There exists a self-adjoint operator called the Hamiltonian, given by

$$H = -\frac{\hbar^2}{2m}\Delta + V(r),$$

whose eigenvalues are called energies. The time evolution of the wave function satisfies the partial differential equation,

$$i\hbar \frac{\partial \psi}{\partial t} = H\psi.$$

Usually, the time-dependence is easy to deal with. Suppose we knew the eigenfunctions of the Hamiltonian,

$$Hu_k = E_k u_k.$$

Then, expanding the wave function in this basis,

$$\psi(\mathbf{r}, t) = \sum_{k=1}^{\infty} a_k(t) u_k(\mathbf{r}),$$

we substitute in the Schrodinger equation and obtain

$$i\hbar \frac{d}{dt} a_k = E_k a_k,$$

i.e.,

$$a_k(t) = a_k(0)\, e^{-\frac{i}{\hbar} E_k t},$$

hence

$$\psi(\mathbf{r}, t) = \sum_{k=1}^{\infty} a_k(0)\, e^{-\frac{i}{\hbar} E_k t} u_k(\mathbf{r}),$$

Moreover, setting $t = 0$ and taking an inner product with u_j we get that

$$a_j(0) = (u_j, \psi(\cdot, 0)).$$

Thus, solving the eigenvalue problem for the Hamiltonian provides at once a solution for the Schrodinger equation.

10.3 A particle in a potential well

As a warmup exercise, consider the case of a particle moving in one space dimension under the influence of a potential,

$$V(x) = \begin{cases} -b & -1 < x < 1 \\ 0 & \text{otherwise.} \end{cases}.$$

Since the potential is discontinuous, so is the second-derivative of ψ, but the first derivative should remain continuous. Recall that we need to solve the eigenvalue problem

$$-\frac{\hbar^2}{2m} \psi'' + V(x)\psi = E\psi.$$

The potential is piecewise constant, i.e.,

$$\psi'' = -\frac{2m}{\hbar^2} \times \begin{cases} E+b & -1 < x < 1 \\ E & \text{otherwise.} \end{cases}$$

What are the admissible solutions? In principle, we would like the solution to belong to $\mathscr{H}$. This is the case when the spectrum is discrete, however, for continuous spectra we must allow for s-called ***generalized solutions***, or ***distributions***.

Case I: $E < -b$ The case of $E < -b$ is impossible in a classical system (the total energy cannot be under the potential energy). If $E < -b$ the solution is of the form

$$\psi(x) = \begin{cases} A_1 e^{kx} + A_2 e^{-kx} & x < -1 \\ B_1 e^{qx} + B_2 e^{-qx} & -1 < x < 1 \\ C_1 e^{kx} + C_2 e^{-kx} & x > 1, \end{cases}$$

where

$$k = \frac{\sqrt{2m|E|}}{\hbar} \qquad \text{and} \qquad q = \frac{\sqrt{2m|E+b|}}{\hbar}.$$

Since we must exclude solutions that diverge at $\pm\infty$ it follows that $A_2 = C_1 = 0$. The continuity of the function and its first derivative at $x = \pm 1$ yields a homogeneous linear system for the four remaining coefficients,

$$\begin{aligned} A_1 e^{-k} &= B_1 e^{-q} + B_2 e^{q} \\ C_2 e^{-k} &= B_1 e^{q} + B_2 e^{-q} \\ A_1 k e^{-k} &= B_1 q e^{-q} - B_2 q e^{q} \\ -C_2 k e^{-k} &= B_1 q e^{q} - B_2 q e^{-q}. \end{aligned}$$

For a non-trivial solution to exist the determinant must vanish, that is

$$\begin{bmatrix} -e^{-k} & e^{-q} & e^{q} & 0 \\ 0 & e^{q} & e^{-q} & -e^{-k} \\ -ke^{-k} & qe^{-q} & -qe^{q} & 0 \\ 0 & qe^{q} & -qe^{-q} & ke^{-k} \end{bmatrix} = 0.$$

It takes little algebra to obtain the condition

$$e^{4q}(k+q)^2 - (k-q)^2 = 0,$$

which cannot be satisfied. I.e., quantum mechanics does not allow either energy states below the minimum of the potential.

Case II: $-b < E < 0$ In the classical setting the particle would remain in the well and move there from side to side. Repeating the above analysis we get

$$\psi(x) = \begin{cases} A_1 e^{kx} + A_2 e^{-kx} & x < -1 \\ B_1 e^{iqx} + B_2 e^{-iqx} & -1 < x < 1 \\ C_1 e^{kx} + C_2 e^{-kx} & x > 1, \end{cases}$$

where

$$k = \frac{\sqrt{2m|E|}}{\hbar} \qquad \text{and} \qquad q = \frac{\sqrt{2m(E+b)}}{\hbar}.$$

A non-trivial solution exists if

$$\begin{bmatrix} -e^{-k} & e^{-iq} & e^{iq} & 0 \\ 0 & e^{iq} & e^{-iq} & -e^{-k} \\ -ke^{-k} & iqe^{-iq} & -iqe^{iq} & 0 \\ 0 & iqe^{iq} & -iqe^{-iq} & ke^{-k} \end{bmatrix} = 0,$$

which gives

$$(q + ik)^2 + e^{4iq}(k + iq)^2 = 0,$$

or

$$\left(\frac{k + iq}{k - iq}\right)^2 = e^{4iq}.$$

Both k and q are functions of energy, and this condition implies that E can at most assume a discrete set of values.

There are now two possibilities: either

$$\frac{k + iq}{k - iq} = -e^{2iq},$$

in which case

$$\frac{k^2 - q^2 + 2ikq}{k^2 + q^2} = -e^{2iq}.$$

Note that $k^2 + q^2 = 2mb/\hbar^2 \equiv k_0^2$. Hence, $k^2 = k_0^2 - q^2$ and

$$1 - 2q^2/k_0^2 = -\cos(2q), \qquad \text{and} \qquad q/k_0 = |\sin q|.$$

The second possibility gives $q/k_0 = |\cos q|$. This equation are easily solved graphically. The remarkable results are (1) there always exist at least one such energy state, (2) the number of energy states is finite.

10.4 The harmonic oscillator

A harmonic oscillator is one-dimension corresponds to the hamiltonian system,

$$H\psi = -\frac{\hbar^2}{2m}\psi'' + V(x)\psi.$$

for $V(x) = \frac{1}{2}m\omega^2 x^2$. Recall that "solving the system" means to find the eigenvalues and eigenvectors of H. That is, we need to solve the eigenvalue problem,

$$-\frac{\hbar^2}{2m}\psi'' + \frac{1}{2}m\omega^2 x^2\psi = E\psi.$$

We start with a change of variables, whose goal is to get rid of constants. Define

$$y = \left(\frac{m\omega}{\hbar}\right)^{1/2} x \qquad \text{and} \qquad \psi(x) = \phi\left(\left(\frac{m\omega}{\hbar}\right)^{1/2} y\right).$$

Substituting, the eigenvalue problem becomes

$$H\phi = -\frac{1}{2}\phi'' + \frac{1}{2}y^2\phi = \frac{E}{\hbar\omega}\phi.$$

The question is for what values of $\lambda = E/\hbar\omega$ this eigenvalue has a solution (in L^2 if the spectrum is discrete and distribution-valued otherwise).

Proposition 10.1 *The eigenvalues of H are non-negative.*

Proof: Let the pair (λ, u) solve the eigenvalue system,

$$-\frac{1}{2}u'' + \frac{1}{2}y^2 u = \lambda u.$$

Multiplying by u^* and integrating over $\mathbb{R}$ we get, after integration by parts,

$$\frac{1}{2}(u', u') + \frac{1}{2}(yu, y, u) = \lambda(u, u),$$

which at once implies that $\lambda \geq 0$. ■

Proposition 10.2 *$\lambda = 1/2$ is an eigenvalue.*

Proof: Take

$$\phi(y) = e^{-y^2/2}.$$

Then,

$$\phi' = -y\phi, \qquad \text{and} \qquad \phi'' = y^2\phi - \phi,$$

so that

$$-\frac{1}{2}\phi'' + \frac{1}{2}y^2\phi = \frac{1}{2}\phi.$$

■

Define now that following two operator,

$$(Y\phi)(y) = y\,\phi(y) \qquad \text{and} \qquad (P\phi)(y) = -i\phi'(y).$$

Note that $H = \frac{1}{2}(P^2 + Y^2)$ (this is an equation between operators), and the commutator of Y and P is given by

$$[Y, P] = YP - PY = -i(y\partial - \partial y) = i.$$

We also define the following two additional operators,

$$A^{\pm} = \frac{1}{\sqrt{2}}(Y \mp iP).$$

and note that

$$[A^+, A^-] = \frac{1}{2}(Y - iP)(Y + iP) - \frac{1}{2}(Y + iP)(Y - iP) = i[Y, P] = i^2 = -1,$$

and

$$A^+A^- = \frac{1}{2}P^2 + \frac{1}{2}Y^2 + \frac{i}{2}[Y, P] = H - \frac{1}{2},$$

so that

$$H = N + \frac{1}{2},$$

where $N = A^+A^-$. Finally,

$$= [A^+A^-, A^+] = A^+A^-A^+ - A^+A^+A^- = A^+$$
$$[N, A^-] = [A^+A^-, A^-] = A^+A^-A^- - A^-A^+A^- = -A^-.$$

Note that the eigenfunction of H are also eigenfunctions of N, and the eigenvalues of H are greater by an half from than the eigenvalues of N. We already know that 0 is an eigenvalue of N.

Suppose now that (λ_k, ϕ_k) are eigensolutions of N, and consider the following indentities,

$$N(A^+\phi_k) = (A^+N + A^+)\phi_k = (\lambda_k + 1)A^+\phi_k.$$

That is, $A^+\phi_k$ is also an eigenfunction with eigenvalue $\lambda_k + 1$. Similarly,

$$N(A^-\phi_k) = (A^-N - A^-)\phi_k = (\lambda_k - 1)A^-\phi_k,$$

i.e., $A^-\phi_k$ is an eigenfunction with eigenvalue $\lambda_k - 1$.

Finally,

$$(A^-\phi_k, A^-\phi_k) = (N\phi_k, \phi) = \lambda_k(\phi_k, \phi_k).$$

I.e., $A_-\phi_0 = 0$.

Bottom line: the eigenvalues of the Hamiltonian are

$$E = \hbar\omega\left(n + \frac{1}{2}\right).$$

Bibliography

[Bar96] G.I. Barenblatt, *Scaling, self-similarity and intermediate asymptotics*, Cambridge University Press, Cambridge, 1996.