Classical Mechanics

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Contents

Chapter 1

Particle Kinematics

1.1 Introduction

Classical mechanics, narrowly defined, is the investigation of the motion of systems of particles in Euclidean three-dimensional space, under the influence of specified force laws, with the motion's evolution determined by Newton's second law, a second order differential equation. That is, given certain laws determining physical forces, and some boundary conditions on the positions of the particles at some particular times, the problem is to determine the positions of all the particles at all times. We will be discussing motions under specific fundamental laws of great physical importance, such as Coulomb's law for the electrostatic force between charged particles. We will also discuss laws which are less fundamental, because the motion under them can be solved explicitly, allowing them to serve as very useful models for approximations to more complicated physical situations, or as a testbed for examining concepts in an explicitly evaluatable situation. Techniques suitable for broad classes of force laws will also be developed.

The formalism of Newtonian classical mechanics, together with investigations into the appropriate force laws, provided the basic framework for physics from the time of Newton until the beginning of this century. The systems considered had a wide range of complexity. One might consider a single particle on which the Earth's gravity acts. But one could also consider systems as the limit of an infinite number of

very small particles, with displacements smoothly varying in space, which gives rise to the continuum limit. One example of this is the consideration of transverse waves on a stretched string, in which every point on the string has an associated degree of freedom, its transverse displacement.

The scope of classical mechanics was broadened in the 19th century, in order to consider electromagnetism. Here the degrees of freedom were not just the positions in space of charged particles, but also other quantities, distributed throughout space, such as the the electric field at each point. This expansion in the type of degrees of freedom has continued, and now in fundamental physics one considers many degrees of freedom which correspond to no spatial motion, but one can still discuss the classical mechanics of such systems.

As a fundamental framework for physics, classical mechanics gave way on several fronts to more sophisticated concepts in the early 1900's. Most dramatically, quantum mechanics has changed our focus from specific solutions for the dynamical degrees of freedom as a function of time to the wave function, which determines the probabilities that a system have particular values of these degrees of freedom. Special relativity not only produced a variation of the Galilean invariance implicit in Newton's laws, but also is, at a fundamental level, at odds with the basic ingredient of classical mechanics — that one particle can exert a force on another, depending only on their simultaneous but different positions. Finally general relativity brought out the narrowness of the assumption that the coordinates of a particle are in a Euclidean space, indicating instead not only that on the largest scales these coordinates describe a curved manifold rather than a flat space, but also that this geometry is itself a dynamical field.

Indeed, most of 20th century physics goes beyond classical Newtonian mechanics in one way or another. As many readers of this book expect to become physicists working at the cutting edge of physics research, and therefore will need to go beyond classical mechanics, we begin with a few words of justification for investing effort in understanding classical mechanics.

First of all, classical mechanics is still very useful in itself, and not just for engineers. Consider the problems (scientific — not political) that NASA faces if it wants to land a rocket on a planet. This requires

an accuracy of predicting the position of both planet and rocket far beyond what one gets assuming Kepler's laws, which is the motion one predicts by treating the planet as a point particle influenced only by the Newtonian gravitational field of the Sun, also treated as a point particle. NASA must consider other effects, and either demonstrate that they are ignorable or include them into the calculations. These include

- multipole moments of the sun
- forces due to other planets
- effects of corrections to Newtonian gravity due to general relativity
- friction due to the solar wind and gas in the solar system

Learning how to estimate or incorporate such effects is not trivial.

Secondly, classical mechanics is not a dead field of research — in fact, in the last two decades there has been a great deal of interest in "dynamical systems". Attention has shifted from calculation of the orbit over fixed intervals of time to questions of the long-term stability of the motion. New ways of looking at dynamical behavior have emerged, such as chaos and fractal systems.

Thirdly, the fundamental concepts of classical mechanics provide the conceptual framework of quantum mechanics. For example, although the Hamiltonian and Lagrangian were developed as sophisticated techniques for performing classical mechanics calculations, they provide the basic dynamical objects of quantum mechanics and quantum field theory respectively. One view of classical mechanics is as a steepest path approximation to the path integral which describes quantum mechanics. This integral over paths is of a classical quantity depending on the "action" of the motion.

So classical mechanics is worth learning well, and we might as well jump right in.

1.2 Single Particle Kinematics

We start with the simplest kind of system, a single unconstrained particle, free to move in three dimensional space, under the influence of a force $\vec{F}$.

1.2.1 Motion in configuration space

The motion of the particle is described by a function which gives its position as a function of time. These positions are points in Euclidean space. Euclidean space is similar to a vector space, except that there is no special point which is fixed as the origin. It does have a metric, that is, a notion of distance between any two points, $D(A, B)$. It also has the concept of a displacement $A - B$ from one point B in the Euclidean space to another, A. These displacements do form a vector space, and for a three-dimensional Euclidean space, the vectors form a three-dimensional real vector space $\mathbb{R}^3$, which can be given an orthonormal basis such that the distance between A and B is given by $D(A, B) = \sum_{i=1}^{3}[(A - B)_i]^2$. Because the mathematics of vector spaces is so useful, we often convert our Euclidean space to a vector space by choosing a particular point as the origin. Each particle's position is then equated to the displacement of that position from the origin, so that it is described by a position vector $\vec{r}$ relative to this origin. But the origin has no physical significance unless it has been choosen in some physically meaningful way. In general the multiplication of a position vector by a scalar is as meaningless physically as saying that 42nd street is three times 14th street. The cartesian components of the vector $\vec{r}$, with respect to some fixed though arbitrary coordinate system, are called the coordinates, cartesian coordinates in this case. We shall find that we often (even usually) prefer to change to other sets of coordinates, such as polar or spherical coordinates, but for the time being we stick to cartesian coordinates.

The motion of the particle is the function $\vec{r}(t)$ of time. Certainly one of the central questions of classical mechanics is to determine, given the physical properties of a system and some initial conditions, what the subsequent motion is. The required "physical properties" is a specification of the force, $\vec{F}$. The beginnings of modern classical mechanics

was the realization at early in the 17th century that the physics, or dynamics, enters into the motion (or kinematics) through the force and its effect on the acceleration, and not through any direct effect of dynamics on the position or velocity of the particle.

Most likely the force will depend on the position of the particle, say for a particle in the gravitational field of a fixed (heavy) source at the origin, for which

$$\vec{F}(\vec{r}) = -\frac{GMm}{r^3}\vec{r}. \tag{1.1}$$

But the force might also depend explicitly on time. For example, for the motion of a spaceship near the Earth, we might assume that the force is given by sum of the Newtonian gravitational forces of the Sun, Moon and Earth. Each of these forces depends on the positions of the corresponding heavenly body, which varies with time. The assumption here is that the motion of these bodies is independent of the position of the light spaceship. We assume someone else has already performed the nontrivial problem of finding the positions of these bodies as functions of time. Given that, we can write down the force the spaceship feels at time t if it happens to be at position $\vec{r}$,

$$\begin{aligned}\vec{F}(\vec{r},t) &= -GmM_S\frac{\vec{r}-\vec{R}_S(t)}{|r-R_S(t)|^3} - GmM_E\frac{\vec{r}-\vec{R}_E(t)}{|r-R_E(t)|^3} \\ &\quad -GmM_M\frac{\vec{r}-\vec{R}_M(t)}{|r-R_M(t)|^3}.\end{aligned}$$

Finally, the force might depend on the velocity of the particle, as for example for the Lorentz force on a charged particle in electric and magnetic fields

$$\vec{F}(\vec{r},\vec{v},t) = q\,\vec{E}(\vec{r},t) + q\,\vec{v}\times\vec{B}(\vec{r},t). \tag{1.2}$$

However the force is determined, it determines the motion of the particle through the second order differential equation known as Newton's Second Law

$$\vec{F}(\vec{r},\vec{v},t) = m\vec{a} = m\frac{d^2\vec{r}}{dt^2}.$$

As this is a second order differential equation, the solution depends in general on two arbitrary (3-vector) parameters, which we might choose to be the initial position and velocity, $\vec{r}(0)$ and $\vec{v}(0)$.

For a given physical situation and a given set of initial conditions for the particle, Newton's laws determine the motion $\vec{r}(t)$, which is a curve in **configuration space** parameterized by time t, known as the **trajectory** in configuration space. If we consider the curve itself, independent of how it depends on time, this is called the **orbit** of the particle. For example, the orbit of a planet, in the approximation that it feels only the field of a fixed sun, is an ellipse. That word does not imply any information about the time dependence or parameterization of the curve.

1.2.2 Conserved Quantities

While we tend to think of Newtonian mechanics as centered on Newton's Second Law in the form $\vec{F} = m\vec{a}$, he actually started with the observation that in the absence of a force, there was uniform motion. We would now say that under these circumstances the **momentum** $\vec{p}(t)$ is **conserved**, $d\vec{p}/dt = 0$. In his second law, Newton stated the effect of a force as producing a rate of change of momentum, which we would write as

$$\vec{F} = d\vec{p}/dt,$$

rather than as producing an acceleration $\vec{F} = m\vec{a}$. In focusing on the concept of momentum, Newton emphasized one of the fundamental quantities of physics, useful beyond Newtonian mechanics, in both relativity and quantum mechanics[1]. Only after using the classical relation of momentum to velocity, $\vec{p} = m\vec{v}$, and the assumption that m is constant, do we find the familiar $\vec{F} = m\vec{a}$.

One of the principal tools in understanding the motion of many systems is isolating those quantities which do not change with time. A **conserved quantity** is a function of the positions and momenta, and perhaps explicitly of time as well, $Q(\vec{r}, \vec{p}, t)$, which remains unchanged when evaluated along the actual motion, $dQ(\vec{r}(t), \vec{p}(t), t)/dt = 0$. A

[1]The relationship of momentum to velocity is changed in these extensions, however.

function depending on the positions, momenta, and time is said to be a function on *extended phase space*[2]. When time is not included, the space is called *phase space*. In this language, a conserved quantity is a function on extended phase space with a vanishing total time derivative along any path which describes the motion of the system.

A single particle with no forces acting on it provides a very simple example. As Newton tells us, $\dot{\vec{p}} = d\vec{p}/dt = \vec{F} = 0$, so the momentum is conserved. There are three more conserved quantities $\vec{Q}(\vec{r}, \vec{p}, t) := \vec{r}(t) - t\vec{p}(t)/m$, which have a time rate of change $d\vec{Q}/dt = \dot{\vec{r}} - \vec{p}/m - t\dot{\vec{p}}/m = 0$. These six independent conserved quantities are as many as one could have for a system with a six dimensional phase space, and they completely solve for the motion. Of course this was a very simple system to solve. We now consider a particle under the influence of a force.

Energy

Consider a particle under the influence of an external force $\vec{F}$. In general, the momentum will not be conserved, although if any cartesian component of the force vanishes along the motion, that component of the momentum will be conserved. Also the **kinetic energy**, defined as $T = \frac{1}{2}m\vec{v}^2$, will not in general be conserved, because

$$\frac{dT}{dt} = m\dot{\vec{v}} \cdot \vec{v} = \vec{F} \cdot \vec{v}.$$

As the particle moves from the point $\vec{r}_i$ to the point $\vec{r}_f$ the total change in the kinetic energy is the **work** done by the force $\vec{F}$,

$$\Delta T = \int_{\vec{r}_i}^{\vec{r}_f} \vec{F} \cdot d\vec{r}.$$

If the force law $\vec{F}(\vec{r}, \vec{p}, t)$ applicable to the particle is independent of time and velocity, then the work done will not depend on how quickly the particle moved along the path from $\vec{r}_i$ to $\vec{r}_f$. If in addition the work done is independent of the path taken between these points, so it depends only on the endpoints, then the force is called a **conservative**

[2]Phase space is discussed further in section 1.4.

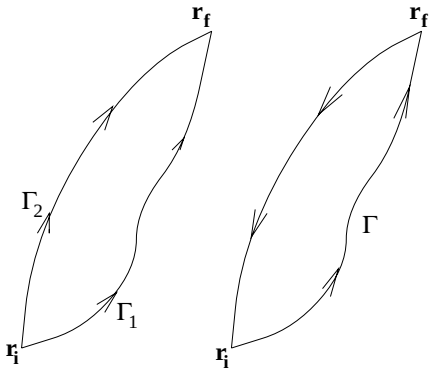
force and we assosciate with it **potential energy**

$$U(\vec{r}) = U(\vec{r}_0) + \int_{\vec{r}}^{\vec{r}_0} \vec{F}(\vec{r}\,') \cdot d\vec{r}\,',$$

where $\vec{r}_0$ is some arbitrary reference position and $U(\vec{r}_0)$ is an arbitrarily chosen reference energy, which has no physical significance in ordinary mechanics. $U(\vec{r})$ represents the potential the force has for doing work on the particle if the particle is at position $\vec{r}$.

The condition for the path integral to be independent of the path is that it gives the same results along any two coterminous paths Γ_1 and Γ_2, or alternatively that it give zero when evaluated along any closed path such as $\Gamma = \Gamma_1 - \Gamma_2$, the path consisting of following Γ_1 and then taking Γ_2 backwards to the starting point. By Stokes' Theorem, this line integral is equivalent to an integral over any surface S bounded by Γ,

$$\oint_\Gamma \vec{F} \cdot d\vec{r} = \int_S \vec{\nabla} \times \vec{F}\, dS.$$



Independence of path $\int_{\Gamma_1} = \int_{\Gamma_2}$ is equivalent to vanishing of the path integral over closed paths Γ, which is in turn equivalent to the vanishing of the curl on the surface whose boundary is Γ.

Thus the requirement that the integral of $\vec{F} \cdot d\vec{r}$ vanish around *any* closed path is equivalent to the requirement that the curl of $\vec{F}$ vanish everywhere in space.

By considering an infinitesimal path from $\vec{r}$ to $\vec{r} + \Delta\vec{r}$, we see that

$$\begin{aligned} U(\vec{r} + \vec{\Delta}) - U(\vec{r}) &= -\vec{F} \cdot \Delta\vec{r}, \quad \text{or} \\ \vec{F}(r) &= -\vec{\nabla} U(r). \end{aligned}$$

The value of the concept of potential energy is that it enables finding a conserved quantity, the total energy, in situtations in which all forces are conservative. Then the total energy $E = T + U$ changes at a rate

$$\frac{dE}{dt} = \frac{dT}{dt} + \frac{d\vec{r}}{dt} \cdot \vec{\nabla} U = \vec{F} \cdot \vec{v} - \vec{v} \cdot \vec{F} = 0.$$

The total energy can also be used in systems with both conservative and nonconservative forces, giving a quantity whose rate of change is determined by the work done only by the nonconservative forces. One example of this usefulness is in the discussion of a slightly damped harmonic oscillator driven by a periodic force near resonance. Then the amplitude of steady-state motion is determined by a balence between the average power input by the driving force and the average power dissipated by friction, the two nonconservative forces in the problem, without needing to worry about the work done by the spring.

Angular momentum

Another quantity which is often useful because it may be conserved is the angular momentum. The definition requires a reference point in the Euclidean space, say $\vec{r}_0$. Then a particle at position $\vec{r}$ with momentum $\vec{p}$ has an **angular momentum** about $\vec{r}_0$ given by $\vec{L} = (\vec{r} - \vec{r}_0) \times \vec{p}$. Very often we take the reference point $\vec{r}_0$ to be the same as the point we have chosen as the origin in converting the Euclidian space to a vector space, so $\vec{r}_0 = 0$, and

$$\begin{aligned} \vec{L} &= \vec{r} \times \vec{p} \\ \frac{d\vec{L}}{dt} &= \frac{d\vec{r}}{dt} \times \vec{p} + \vec{r} \times \frac{d\vec{p}}{dt} = \frac{1}{m}\vec{p} \times \vec{p} + \vec{r} \times \vec{F} = 0 + \vec{\tau} = \vec{\tau}. \end{aligned}$$

where we have defined the **torque** about $\vec{r}_0$ as $\tau = (\vec{r} - \vec{r}_0) \times \vec{F}$ in general, and $\tau = \vec{r} \times \vec{F}$ when our reference point $\vec{r}_0$ is at the origin.

We see that if the torque $\vec{\tau}(t)$ vanishes (at all times) the angular momentum is conserved. This can happen not only if the force is zero, but also if the force always points to the reference point. This is the case in a central force problem such as motion of a planet about the sun.

1.3 Systems of Particles

So far we have talked about a system consisting of only a single particle, possibly influenced by external forces. Consider now a system of n particles with positions $\vec{r}_i$, $i = 1, \ldots, n$, in flat space. The configuration

of the system then has $3n$ coordinates (configuration space is $\mathbb{R}^{3n}$), and the phase space has $6n$ coordinates $\{\vec{r}_i, \vec{p}_i\}$.

1.3.1 External and internal forces

Let $\vec{F}_i$ be the total force acting on particle i. It is the sum of the forces produced by each of the other particles and that due to any external force. Let $\vec{F}_{ji}$ be the force particle j exerts on particle i and let $\vec{F}_i^E$ be the external force on particle i. Using Newton's second law on particle i, we have

$$\vec{F}_i = \vec{F}_i^E + \sum_j \vec{F}_{ji} = \dot{\vec{p}}_i = m_i \dot{\vec{v}}_i,$$

where m_i is the mass of the i'th particle. Here we are assuming forces have identifiable causes, which is the real meaning of Newton's second law, and that the causes are either individual particles or external forces. Thus we are assuming there are no "three-body" forces which are not simply the sum of "two-body" forces that one object exerts on another.

Define the **center of mass** and **total mass**

$$\vec{R} = \frac{\sum m_i \vec{r}_i}{\sum m_i}, \qquad M = \sum m_i.$$

Then if we define the **total momentum**

$$\vec{P} = \sum \vec{p}_i = \sum m_i \vec{v}_i = \frac{d}{dt} \sum m_i \vec{r}_i = M \frac{d\vec{R}}{dt},$$

we have

$$\frac{d\vec{P}}{dt} = \dot{\vec{P}} = \sum \dot{\vec{p}}_i = \sum \vec{F}_i = \sum_i \vec{F}_i^E + \sum_{ij} \vec{F}_{ji}.$$

Let us define $\vec{F}^E = \sum_i F_i^E$ to be the **total external force**. If Newton's Third Law holds,

$$\vec{F}_{ji} = -\vec{F}_{ij}, \text{ so } \sum_{ij} \vec{F}_{ij} = 0, \text{ and}$$

$$\dot{\vec{P}} = \vec{F}^E. \tag{1.3}$$

Thus the internal forces cancel in pairs in their effect on the total momentum, which changes only in response to the total external force. As an obvious but very important consequence[3] *the total momentum of an isolated system is conserved.*

The total angular momentum is also just a sum over the individual particles, in this case of the individual angular momenta:

$$\vec{L} = \sum \vec{L}_i = \sum \vec{r}_i \times \vec{p}_i.$$

Its rate of change with time is

$$\frac{d\vec{L}}{dt} = \dot{\vec{L}} = \sum_i \vec{v}_i \times \vec{p}_i + \sum_i \vec{r}_i \times \vec{F}_i = 0 + \sum \vec{r}_i \times \vec{F}_i^E + \sum_{ij} \vec{r}_i \times \vec{F}_{ji}.$$

The total external torque is naturally defined as

$$\vec{\tau} = \sum_i \vec{r}_i \times \vec{F}_i^E,$$

[3]There are situations and ways of describing them in which the law of action and reaction seems not to hold. For example, a current i_1 flowing through a wire segment $d\vec{s}_1$ contributes, according to the law of Biot and Savart, a magnetic field $d\vec{B} = \mu_0 i_1 d\vec{s}_1 \times \vec{r}/4\pi|r|^3$ at a point $\vec{r}$ away from the current element. If a current i_2 flows through a segment of wire $d\vec{s}_2$ at that point, it feels a force

$$\vec{F}_{12} = \frac{\mu_0}{4\pi} i_1 i_2 \frac{d\vec{s}_2 \times (d\vec{s}_1 \times \vec{r})}{|r|^3}$$

due to element 1. On the other hand $\vec{F}_{21}$ is given by the same expression with $d\vec{s}_1$ and $d\vec{s}_2$ interchanged and the sign of $\vec{r}$ reversed, so

$$\vec{F}_{12} + \vec{F}_{21} = \frac{\mu_0}{4\pi} \frac{i_1 i_2}{|r|^3} \left[d\vec{s}_1 (d\vec{s}_2 \cdot \vec{r}) - d\vec{s}_2 (d\vec{s}_1 \cdot \vec{r}) \right],$$

which is not generally zero.

One should not despair for the validity of momentum conservation. The Law of Biot and Savart only holds for time-independent current distributions. Unless the currents form closed loops, there will be a charge buildup and Coulomb forces need to be considered. If the loops are closed, the total momentum will involve integrals over the two closed loops, for which $\int\int F_{12} + F_{21}$ can be shown to vanish. More generally, even the sum of the momenta of the current elements is not the whole story, because there is momentum in the electromagnetic field, which will be changing in the time-dependent situation.

so we might ask if the last term vanishes due the Third Law, which permits us to rewrite $\vec{F}_{ji} = \frac{1}{2}\left(\vec{F}_{ji} - \vec{F}_{ij}\right)$. Then the last term becomes

$$\begin{aligned}\sum_{ij} \vec{r}_i \times \vec{F}_{ji} &= \frac{1}{2}\sum_{ij} \vec{r}_i \times \vec{F}_{ji} - \frac{1}{2}\sum_{ij} \vec{r}_i \times \vec{F}_{ij} \\ &= \frac{1}{2}\sum_{ij} \vec{r}_i \times \vec{F}_{ji} - \frac{1}{2}\sum_{ij} \vec{r}_j \times \vec{F}_{ji} \\ &= \frac{1}{2}\sum_{ij} (\vec{r}_i - \vec{r}_j) \times \vec{F}_{ji}.\end{aligned}$$

This is not automatically zero, but vanishes if one assumes a stronger form of the Third Law, namely that the action and reaction forces between two particles acts along the line of separation of the particles. If the force law is independent of velocity and rotationally and translationally symmetric, there is no other direction for it to point. For spinning particles and magnetic forces the argument is not so simple — in fact electromagnetic forces between moving charged particles are really only correctly viewed in a context in which the system includes not only the particles but also the fields themselves. For such a system, in general the total energy, momentum, and angular momentum of the particles alone will not be conserved, because the fields can carry all of these quantities. But properly defining the energy, momentum, and angular momentum of the electromagnetic fields, and including them in the totals, will result in quantities conserved as a result of symmetries of the underlying physics. This is further discussed in section 8.1.

Making the assumption that the strong form of Newton's Third Law holds, we have shown that

$$\vec{\tau} = \frac{d\vec{L}}{dt}. \tag{1.4}$$

The conservation laws are very useful because they permit algebraic solution for part of the velocity. Taking a single particle as an example, if $E = \frac{1}{2}mv^2 + U(\vec{r})$ is conserved, the speed $|v(t)|$ is determined at all times (as a function of $\vec{r}$) by one arbitrary constant E. Similarly if $\vec{L}$ is conserved, the components of $\vec{v}$ which are perpendicular to $\vec{r}$ are determined in terms of the fixed constant $\vec{L}$. With both conserved, $\vec{v}$

is completely determined except for the sign of the radial component. Examples of the usefulness of conserved quantities are everywhere, and will be particularly clear when we consider the two body central force problem later. But first we continue our discussion of general systems of particles.

As we mentioned earlier, the total angular momentum depends on the point of evaluation, that is, the origin of the coordinate system used. We now show that it consists of two contributions, the angular momentum about the center of mass and the angular momentum of a fictitious point object located at the center of mass. Let $\vec{r}\,'_i$ be the position of the i'th particle with respect to the center of mass, so $\vec{r}\,'_i = \vec{r}_i - \vec{R}$. Then

$$\begin{aligned}
\vec{L} &= \sum_i m_i \vec{r}_i \times \vec{v}_i = \sum_i m_i \left(\vec{r}\,'_i + \vec{R}\right) \times \left(\dot{\vec{r}}\,'_i + \dot{\vec{R}}\right) \\
&= \sum_i m_i \vec{r}\,'_i \times \dot{\vec{r}}\,'_i + \sum_i m_i \vec{r}\,'_i \times \dot{\vec{R}} \\
&\qquad + \vec{R} \times \sum m_i \dot{\vec{r}}\,'_i + M\vec{R} \times \dot{\vec{R}} \\
&= \sum_i \vec{r}\,'_i \times \vec{p}\,'_i + \vec{R} \times \vec{P}.
\end{aligned}$$

Here we have noted that $\sum m_i \vec{r}\,'_i = 0$, and also its derivative $\sum m_i \vec{v}\,'_i = 0$. We have defined $\vec{p}\,'_i = m_i \vec{v}\,'_i$, the momentum in the center of mass reference frame. The first term of the final form is the sum of the angular momenta of the particles *about their center of mass*, while the second term is the angular momentum the system would have if it were collapsed to a point at the center of mass.

What about the total energy? The kinetic energy

$$\begin{aligned}
T &= \frac{1}{2}\sum m_i v_i^2 = \frac{1}{2}\sum m_i \left(\vec{v}\,'_i + \vec{V}\right) \cdot \left(\vec{v}\,'_i + \vec{V}\right) \\
&= \frac{1}{2}\sum m_i v'^2_i + \frac{1}{2}MV^2, \qquad (1.5)
\end{aligned}$$

where the cross term vanishes, once again, because $\sum m_i \vec{v}\,'_i = 0$. Thus the kinetic energy of the system can also be viewed as the sum of the kinetic energies of the constituents about the center of mass, plus the

kinetic energy the system would have if it were collapsed to a particle at the center of mass.

If the forces on the system are due to potentials, the total energy will be conserved, but this includes not only the potential due to the external forces but also that due to interparticle forces, $\sum U_{ij}(\vec{r}_i, \vec{r}_j)$. In general this contribution will not be zero or even constant with time, and the internal potential energy will need to be considered. One exception to this is the case of a rigid body.

1.3.2 Constraints

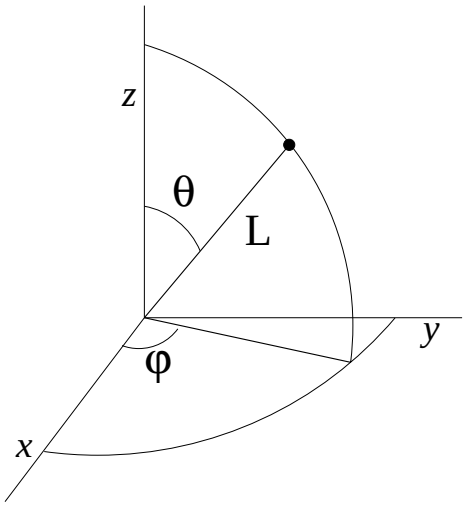
A rigid body is defined as a system of n particles for which all the interparticle distances are constrained to fixed constants, $|\vec{r}_i - \vec{r}_j| = c_{ij}$, and the interparticle potentials are functions only of these interparticle distances. As these distances do not vary, neither does the internal potential energy. These interparticle forces cannot do work, and the internal potential energy may be ignored.

The rigid body is an example of a constrained system, in which the general $3n$ degrees of freedom are restricted by some forces of constraint which place conditions on the coordinates $\vec{r}_i$, perhaps in conjunction with their momenta. In such descriptions we do not wish to consider or specify the forces themselves, but only their (approximate) effect. The forces are assumed to be whatever is necessary to have that effect. It is generally assumed, as in the case with the rigid body, that the constraint forces do no work under displacements allowed by the constraints. We will consider this point in more detail later.

If the constraints can be phrased so that they are on the coordinates and time only, as $\Phi_i(\vec{r}_1, ...\vec{r}_n, t) = 0, i = 1, \ldots, k$, they are known as **holonomic constraints**. These constraints determine hypersurfaces in configuration space to which all motion of the system is confined. In general this hypersurface forms a $3n - k$ dimensional manifold. We might describe the configuration point on this manifold in terms of $3n - k$ generalized coordinates, $q_j, j = 1, \ldots, 3n - k$, so that the $3n - k$ variables q_j, together with the k constraint conditions $\Phi_i(\{\vec{r}_i\}) = 0$, determine the $\vec{r}_i = \vec{r}_i(q_1, \ldots, q_{3n-k}, t)$

The constrained subspace of configuration space need not be a flat space. Consider, for example, a mass on one end of a rigid light rod

of length L, the other end of which is fixed to be at the origin $\vec{r} = 0$, though the rod is completely free to rotate. Clearly the possible values of the cartesian coordinates $\vec{r}$ of the position of the mass satisfy the constraint $|\vec{r}| = L$, so $\vec{r}$ lies on the surface of a sphere of radius L. We might choose as generalized coordinates the standard spherical angles θ and ϕ. Thus the constrained subspace is two dimensional but not flat — rather it is the surface of a sphere, which mathematicians call S^2. It is natural to reexpress the dynamics in terms of θ and ϕ.



Generalized coordinates (θ, ϕ) for a particle constrained to lie on a sphere.

The use of generalized (non-cartesian) coordinates is not just for constrained systems. The motion of a particle in a central force field about the origin, with a potential $U(\vec{r}) = U(|\vec{r}|)$, is far more naturally described in terms of spherical coordinates r, θ, and ϕ than in terms of x, y, and z.

Before we pursue a discussion of generalized coordinates, it must be pointed out that not all constraints are holonomic. The standard example is a disk of radius R, which rolls on a fixed horizontal plane. It is constrained to always remain vertical, and also to roll without slipping on the plane. As coordinates we can choose the x and y of the center of the disk, which are also the x and y of the contact point, together with the angle a fixed line on the disk makes with the downward direction, ϕ, and the angle the axis of the disk makes with the x axis, θ.

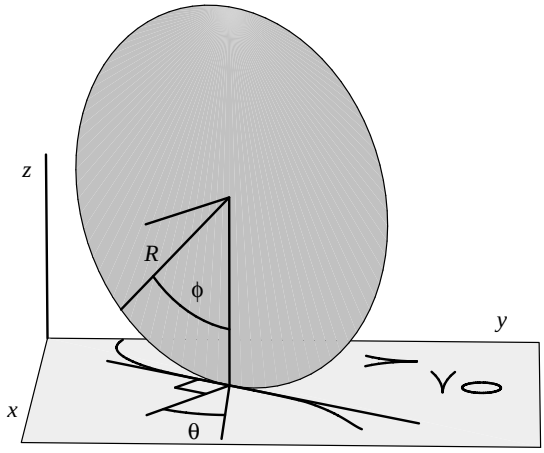
As the disk rolls through an angle $d\phi$, the point of contact moves a distance $Rd\phi$ in a direction depending on θ,

$$\begin{aligned} Rd\phi\sin\theta &= dx \\ Rd\phi\cos\theta &= dy \end{aligned}$$

Dividing by dt, we get two constraints involving the positions *and* velocities,

$$\begin{aligned} \Phi_1 &:= R\dot{\phi}\sin\theta - \dot{x} = 0 \\ \Phi_2 &:= R\dot{\phi}\cos\theta - \dot{y} = 0. \end{aligned}$$

The fact that these involve velocities does not automatically make them nonholonomic. In the simpler one-dimensional problem in which the disk is confined to the yz plane, rolling along $x = 0$ ($\theta = 0$), we would have only the coordinates ϕ and y, with the rolling constraint $R\dot{\phi} - \dot{y} = 0$. But this constraint can be integrated, $R\phi(t) - y(t) = c$, for some constant c, so that it becomes a constraint among just the coordinates, and is holomorphic. This cannot be done with the two-dimensional problem. We can see that there is no constraint among the four coordinates themselves because each of them can be changed by a motion which leaves the others unchanged. Rotating θ without moving the other coordinates is straightforward. By rolling the disk along each of the three small paths shown to the right of the disk, we can change one of the variables x, y, or ϕ, respectively, with no net change in the other coordinates. Thus all values of the coordinates[4] can be achieved in this fashion.



A vertical disk free to roll on a plane. A fixed line on the disk makes an angle of ϕ with respect to the vertical, and the axis of the disk makes an angle θ with the x-axis. The long curved path is the trajectory of the contact point. The three small paths are alternate trajectories illustrating that x, y, and ϕ can each be changed without any net change in the other coordinates.

[4]Thus the configuration space is $x \in \mathbb{R}$, $y \in \mathbb{R}$, $\theta \in [0, 2\pi)$ and $\phi \in [0, 2\pi)$,

There are other, less interesting, nonholonomic constraints given by inequalities rather than constraint equations. A bug sliding down a bowling ball obeys the constraint $|\vec{r}| \geq R$. Such problems are solved by considering the constraint with an equality ($|\vec{r}| = R$), but restricting the region of validity of the solution by an inequality on the constraint force ($N \geq 0$), and then supplementing with the unconstrained problem once the bug leaves the surface.

In quantum field theory, anholonomic constraints which are functions of the positions and momenta are further subdivided into first and second class constraints *à la* Dirac, with the first class constraints leading to local gauge invariance, as in Quantum Electrodynamics or Yang-Mills theory. But this is heading far afield.

1.3.3 Generalized Coordinates for Unconstrained Systems

Before we get further into constrained systems and D'Alembert's Principle, we will discuss the formulation of a conservative unconstrained system in generalized coordinates. Thus we wish to use $3n$ generalized coordinates q_j, which, together with time, determine all of the $3n$ cartesian coordinates $\vec{r}_i$:

$$\vec{r}_i = \vec{r}_i(q_1, ..., q_{3n}, t).$$

Notice that this is a relationship between different descriptions of the same point in configuration space, and the functions $\vec{r}_i(\{q\}, t)$ are independent of the motion of any particle. We are assuming that the $\vec{r}_i$ and the q_j are each a complete set of coordinates for the space, so the q's are also functions of the $\{\vec{r}_i\}$ and t:

$$q_j = q_j(\vec{r}_1, ..., \vec{r}_n, t).$$

The t dependence permits there to be an explicit dependence of this relation on time, as we would have, for example, in relating a rotating coordinate system to an inertial cartesian one.

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or, if we allow more carefully for the continuity as θ and ϕ go through 2π, the more accurate statement is that configuration space is $\mathbb{R}^2 \times (S^1)^2$, where S^1 is the circumference of a circle, $\theta \in [0, 2\pi]$, with the requirement that $\theta = 0$ is equivalent to $\theta = 2\pi$.

Let us change the cartesian coordinate notation slightly, with $\{x_k\}$ the $3n$ cartesian coordinates of the n 3-vectors $\vec{r}_i$, deemphasizing the division of these coordinates into triplets.

A small change in the coordinates of a particle in configuration space, whether an actual change over a small time interval dt or a "virtual" change between where a particle is and where it might have been under slightly altered circumstances, can be described by a set of δx_k or by a set of δq_j. If we are talking about a virtual change at the same time, these are related by the chain rule

$$\delta x_k = \sum_j \frac{\partial x_k}{\partial q_j}\delta q_j, \quad \delta q_j = \sum_k \frac{\partial q_j}{\partial x_k}\delta x_k, \quad (\text{for } \delta t = 0). \tag{1.6}$$

For the actual motion through time, or any variation where δt is not assumed to be zero, we need the more general form,

$$\delta x_k = \sum_j \frac{\partial x_k}{\partial q_j}\delta q_j + \frac{\partial x_k}{\partial t}\delta t, \quad \delta q_j = \sum_k \frac{\partial q_j}{\partial x_k}\delta x_k + \frac{\partial q_k}{\partial t}\delta t. \tag{1.7}$$

A virtual displacement, with $\delta t = 0$, is the kind of variation we need to find the forces described by a potential. Thus the force is

$$F_k = -\frac{\partial U(\{x\})}{\partial x_k} = -\sum_j \frac{\partial U(\{x(\{q\})\})}{\partial q_j}\frac{\partial q_j}{\partial x_k} = \sum_j \frac{\partial q_j}{\partial x_k}Q_j, \tag{1.8}$$

where

$$Q_j := \sum_k F_k \frac{\partial x_k}{\partial q_j} = -\frac{\partial U(\{x(\{q\})\})}{\partial q_j} \tag{1.9}$$

is known as the **generalized force**. We may think of $\tilde{U}(q,t) := U(x(q),t)$ as a potential in the generalized coordinates $\{q\}$. Note that if the coordinate transformation is time-dependent, it is possible that a time-independent potential $U(x)$ will lead to a time-dependent potential $\tilde{U}(q,t)$, and a system with forces described by a time-dependent potential is not conservative.

The definition in (1.9) of the generalized force Q_j holds even if the cartesian force is not described by a potential.

The q_k do not necessarily have units of distance. For example, one q_k might be an angle, as in polar or spherical coordinates. The corresponding component of the generalized force will have the units of energy and we might consider it a torque rather than a force.

1.3.4 Kinetic energy in generalized coordinates

We have seen that, under the right circumstances, the potential energy can be thought of as a function of the generalized coordinates q_k, and the generalized forces Q_k are given by the potential just as for ordinary cartesian coordinates and their forces. Now we examine the kinetic energy

$$T = \frac{1}{2}\sum_i m_i \dot{\vec{r}}_i^{\,2} = \frac{1}{2}\sum_j m_j \dot{x}_j^2$$

where the $3n$ values m_j are not really independent, as each particle has the same mass in all three dimensions in ordinary Newtonian mechanics[5]. Now

$$\dot{x}_j = \lim_{\Delta t\to 0}\frac{\Delta x_j}{\Delta t} = \lim_{\Delta t\to 0}\left(\sum_k \left.\frac{\partial x_j}{\partial q_k}\right|_{q,t}\frac{\Delta q_k}{\Delta t}\right) + \left.\frac{\partial x_j}{\partial t}\right|_q,$$

where $|_{q,t}$ means that t and the q's other than q_k are held fixed. The last term is due to the possibility that the coordinates $x_i(q_1, ..., q_{3n}, t)$ may vary with time even for fixed values of q_k. So the chain rule is giving us

$$\dot{x}_j = \frac{dx_j}{dt} = \sum_k \left.\frac{\partial x_j}{\partial q_k}\right|_{q,t}\dot{q}_k + \left.\frac{\partial x_j}{\partial t}\right|_q. \tag{1.10}$$

Plugging this into the kinetic energy, we see that

$$T = \frac{1}{2}\sum_{j,k,\ell} m_j \frac{\partial x_j}{\partial q_k}\frac{\partial x_j}{\partial q_\ell}\dot{q}_k\dot{q}_\ell + \sum_{j,k} m_j \frac{\partial x_j}{\partial q_k}\dot{q}_k \left.\frac{\partial x_j}{\partial t}\right|_q + \frac{1}{2}\sum_j m_j \left(\left.\frac{\partial x_j}{\partial t}\right|_q\right)^2. \tag{1.11}$$

What is the interpretation of these terms? Only the first term arises if the relation between x and q is time independent. The second and third terms are the sources of the $\dot{\vec{r}}\cdot(\vec{\omega}\times\vec{r})$ and $(\vec{\omega}\times\vec{r})^2$ terms in the kinetic energy when we consider rotating coordinate systems[6].

[5] But in an anisotropic crystal, the effective mass of a particle might in fact be different in different directions.

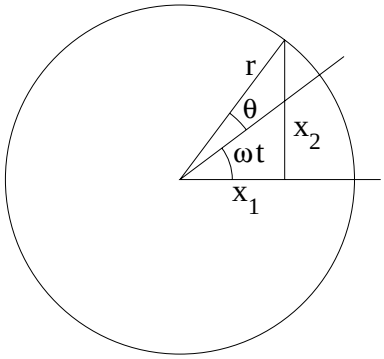
[6] This will be fully developed in section 4.2

Let's work a simple example: we will consider a two dimensional system using polar coordinates with θ measured from a direction rotating at angular velocity ω. Thus the angle the radius vector to an arbitrary point (r, θ) makes with the inertial x_1-axis is $\theta + \omega t$, and the relations are

$$\begin{aligned} x_1 &= r\cos(\theta + \omega t), \\ x_2 &= r\sin(\theta + \omega t), \end{aligned}$$

with inverse relations

$$\begin{aligned} r &= \sqrt{x_1^2 + x_2^2}, \\ \theta &= \sin^{-1}(x_2/r) - \omega t. \end{aligned}$$



Rotating polar coordinates related to inertial cartesian coordinates.

So $\dot{x}_1 = \dot{r}\cos(\theta+\omega t) - \dot{\theta} r \sin(\theta+\omega t) - \omega r \sin(\theta+\omega t)$, where the last term is from $\partial x_j/\partial t$, and $\dot{x}_2 = \dot{r}\sin(\theta+\omega t) + \dot{\theta} r\cos(\theta+\omega t) + \omega r\cos(\theta+\omega t)$. In the square, things get a bit simpler, $\sum \dot{x}_i^2 = \dot{r}^2 + r^2(\omega + \dot{\theta})^2$.

We see that the form of the kinetic energy in terms of the generalized coordinates and their velocities is much more complicated than it is in cartesian inertial coordinates, where it is coordinate independent, and a simple diagonal quadratic form in the velocities. In generalized coordinates, it is quadratic but not homogeneous[7] in the velocities, and with an arbitrary dependence on the coordinates. In general, even if the coordinate transformation is time **independent**, the form of the kinetic energy is still coordinate dependent and, while a purely quadratic form in the velocities, it is not necessarily diagonal. In this time-independent situation, we have

$$T = \frac{1}{2}\sum_{k\ell} M_{k\ell}\dot{q}_k\dot{q}_\ell, \qquad \text{with} \qquad M_{k\ell} = \sum_j m_j \frac{\partial x_j}{\partial q_k}\frac{\partial x_j}{\partial q_\ell}, \tag{1.12}$$

where $M_{k\ell}$ is known as the mass matrix, and is always symmetric but not necessarily diagonal or coordinate independent.

[7] It involves quadratic and lower order terms in the velocities, not just quadratic ones.

The mass matrix is independent of the $\partial x_j/\partial t$ terms, and we can understand the results we just obtained for it in our two-dimensional example above,

$$M_{11} = m, \qquad M_{12} = M_{21} = 0, \qquad M_{22} = mr^2,$$

by considering the case without rotation, $\omega = 0$. We can also derive this expression for the kinetic energy in nonrotating polar coordinates by expressing the velocity vector $\vec{v} = \dot{r}\hat{e}_r + r\dot{\theta}\hat{e}_\theta$ in terms of unit vectors in the radial and tangential directions respectively. The coefficients of these unit vectors can be understood graphically with geometric arguments. This leads more quickly to $\vec{v}^2 = (\dot{r})^2 + r^2(\dot{\theta})^2$, $T = \frac{1}{2}m\dot{r}^2 + \frac{1}{2}mr^2\dot{\theta}^2$, and the mass matrix follows. Similar geometric arguments are usually used to find the form of the kinetic energy in spherical coordinates, but the formal approach of (1.12) enables us to find the form even in situations where the geometry is difficult to picture.

It is important to keep in mind that when we view T as a function of coordinates and velocities, these are independent arguments evaluated at a particular moment of time. Thus we can ask independently how T varies as we change x_i or as we change $\dot{x}_i$, each time holding the other variable fixed. Thus the kinetic energy is not a function on the $3n$-dimensional configuration space, but on a larger, $6n$-dimensional space[8] with a point specifying both the coordinates $\{q_i\}$ and the velocities $\{\dot{q}_i\}$.

1.4 Phase Space

If the trajectory of the system in configuration space, $\vec{r}(t)$, is known, the velocity as a function of time, $\vec{v}(t)$ is also determined. As the mass of the particle is simply a physical constant, the momentum $\vec{p} = m\vec{v}$ contains the same information as the velocity. Viewed as functions of time, this gives nothing beyond the information in the trajectory. But at any given time, $\vec{r}$ and $\vec{p}$ provide a complete set of initial conditions, while $\vec{r}$ alone does not. We define **phase space** as the set of possible positions

[8]This space is called the tangent bundle to configuration space. For cartesian coordinates it is almost identical to phase space, which is in general the "**cotangent bundle**" to configuration space.

and momenta for the system at some instant. Equivalently, it is the set of possible initial conditions, or the set of possible motions obeying the equations of motion. For a single particle in cartesian coordinates, the six coordinates of phase space are the three components of $\vec{r}$ and the three components of $\vec{p}$. At any instant of time, the system is represented by a point in this space, called the **phase point**, and that point moves with time according to the physical laws of the system. These laws are embodied in the force function, which we now consider as a function of $\vec{p}$ rather than $\vec{v}$, in addition to $\vec{r}$ and t. We may write these equations as

$$\begin{aligned} \frac{d\vec{r}}{dt} &= \frac{\vec{p}}{m}, \\ \frac{d\vec{p}}{dt} &= \vec{F}(\vec{r}, \vec{p}, t). \end{aligned}$$

Note that these are first order equations, which means that the motion of the point representing the system in phase space is completely determined[9] by where the phase point is. This is to be distinguished from the trajectory in configuration space, where in order to know the trajectory you must have not only an initial point (position) but also an initial velocity.

1.4.1 Dynamical Systems

We have spoken of the coordinates of phase space for a single particle as $\vec{r}$ and $\vec{p}$, but from a mathematical point of view these together give the coordinates of the phase point in phase space. We might describe these coordinates in terms of a six dimensional vector $\vec{\eta} = (r_1, r_2, r_3, p_1, p_2, p_3)$. The physical laws determine at each point a **velocity function** for the phase point as it moves through phase space,

$$\frac{d\vec{\eta}}{dt} = \vec{V}(\vec{\eta}, t), \tag{1.13}$$

which gives the velocity at which the phase point representing the system moves through phase space. Only half of this velocity is the ordi-

[9] We will assume throughout that the force function is a well defined continuous function of its arguments.

nary velocity, while the other half represents the rapidity with which the momentum is changing, *i.e.* the force. The path traced by the phase point as it travels through phase space is called the **phase curve**.

For a system of n particles in three dimensions, the complete set of initial conditions requires $3n$ spatial coordinates and $3n$ momenta, so phase space is $6n$ dimensional. While this certainly makes visualization difficult, the large dimensionality is no hindrance for formal developments. Also, it is sometimes possible to focus on particular dimensions, or to make generalizations of ideas familiar in two and three dimensions. For example, in discussing integrable systems (7.1), we will find that the motion of the phase point is confined to a $3n$-dimensional torus, a generalization of one and two dimensional tori, which are circles and the surface of a donut respectively.

Thus for a system composed of a finite number of particles, the dynamics is determined by the first order ordinary differential equation (1.13), formally a very simple equation. All of the complication of the physical situation is hidden in the large dimensionality of the dependent variable $\vec{\eta}$ and in the functional dependence of the velocity function $V(\vec{\eta}, t)$ on it.

There are other systems besides Newtonian mechanics which are controlled by equation (1.13), with a suitable velocity function. Collectively these are known as **dynamical systems**. For example, individuals of an asexual mutually hostile species might have a fixed birth rate b and a death rate proportional to the population, so the population would obey the **logistic equation**[10] $dp/dt = bp - cp^2$, a dynamical system with a one-dimensional space for its dependent variable. The populations of three competing species could be described by eq. (1.13) with $\vec{\eta}$ in three dimensions.

The dimensionality d of $\vec{\eta}$ in (1.13) is called the **order of the dynamical system**. A d'th order differential equation in one independent variable may always be recast as a first order differential equation in d variables, so it is one example of a d'th order dynamical system. The space of these dependent variables is called the phase space of the dynamical system. Newtonian systems always give rise to an even-order

[10]This is not to be confused with the simpler *logistic map*, which is a recursion relation with the same form but with solutions displaying a very different behavior.

system, because each spatial coordinate is paired with a momentum. For n particles unconstrained in D dimensions, the order of the dynamical system is $d = 2nD$. Even for constrained Newtonian systems, there is always a pairing of coordinates and momenta, which gives a restricting structure, called the symplectic structure[11], on phase space.

If the force function does not depend explicitly on time, we say the system is **autonomous**. The velocity function has no explicit dependance on time, $\vec{V} = \vec{V}(\vec{\eta})$, and is a time-independent vector field on phase space, which we can indicate by arrows just as we might the electric field in ordinary space. This gives a visual indication of the motion of the system's point. For example, consider a damped harmonic oscillator with $\vec{F} = -kx - \alpha p$, for which the velocity function is

$$\left(\frac{dx}{dt}, \frac{dp}{dt}\right) = \left(\frac{p}{m}, -kx - \alpha p\right).$$

A plot of this field for the undamped ($\alpha = 0$) and damped oscillators

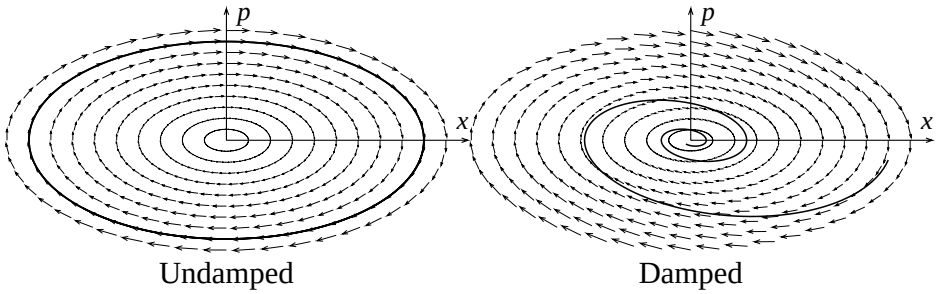


Figure 1.1: Velocity field for undamped and damped harmonic oscillators, and one possible phase curve for each system through phase space.

is shown in Figure 1.1. The velocity field is everywhere tangent to any possible path, one of which is shown for each case. Note that qualitative features of the motion can be seen from the velocity field without any solving of the differential equations; it is clear that in the damped case the path of the system must spiral in toward the origin.

The paths taken by possible physical motions through the phase space of an autonomous system have an important property. Because

[11] This will be discussed in sections (6.3) and (6.6).

the rate and direction with which the phase point moves away from a given point of phase space is completely determined by the velocity function at that point, if the system ever returns to a point it must move away from that point exactly as it did the last time. That is, if the system at time T returns to a point in phase space that it was at at time $t = 0$, then its subsequent motion must be just as it was, so $\vec{\eta}(T + t) = \vec{\eta}(t)$, and the motion is **periodic** with **period** T. This almost implies that the phase curve the object takes through phase space must be nonintersecting[12].

In the non-autonomous case, where the velocity field is time dependent, it may be preferable to think in terms of extended phase space, a $6n+1$ dimensional space with coordinates $(\vec{\eta}, t)$. The velocity field can be extended to this space by giving each vector a last component of 1, as $dt/dt = 1$. Then the motion of the system is relentlessly upwards in this direction, though still complex in the others. For the undamped one-dimensional harmonic oscillator, the path is a helix in the three dimensional extended phase space.

Most of this book is devoted to finding analytic methods for exploring the motion of a system. In several cases we will be able to find exact analytic solutions, but it should be noted that these exactly solvable problems, while very important, cover only a small set of real problems. It is therefore important to have methods other than searching for analytic solutions to deal with dynamical systems. Phase space provides one method for finding qualitative information about the solutions. Another approach is numerical. Newton's Law, and more generally the equation (1.13) for a dynamical system, is a set of ordinary differential equations for the evolution of the system's position in phase space. Thus it is always subject to numerical solution given an initial configuration, at least up until such point that some singularity in the velocity function is reached. One primitive technique which will work for all such systems is to choose a small time interval of length Δt, and use $d\vec{\eta}/dt$ at the beginning of each interval to approximate $\Delta\vec{\eta}$ during this interval. This gives a new approximate value for $\vec{\eta}$ at the

[12] An exception can occur at an unstable equilibrium point, where the velocity function vanishes. The motion can just end at such a point, and several possible phase curves can terminate at that point.

end of this interval, which may then be taken as the beginning of the next.[13]

As an example, we show the meat of a calculation for the damped harmonic oscillator, in Fortran. This same technique will work even with a very complicated situation. One need only add lines for all the components of the position and momentum, and change the force law appropriately.

```
do i = 1,n
  dx = (p/m) * dt
  dp = -(k*x+alpha*p)*dt
  x = x + dx
  p = p + dp
  t = t + dt
  write *, t, x, p
enddo
```

Integrating the motion, for a damped harmonic oscillator.

This is not to say that numerical solution is a good way to solve this problem. An analytical solution, if it can be found, is almost always preferable, because

- It is far more likely to provide insight into the qualitative features of the motion.
- Numerical solutions must be done separately for each value of the parameters (k, m, α) and each value of the initial conditions (x_0 and p_0).
- Numerical solutions have subtle numerical problems in that they are only exact as $\Delta t \to 0$, and only if the computations are done exactly. Sometimes uncontrolled approximate solutions lead to surprisingly large errors.

[13] This is a very unsophisticated method. The errors made in each step for $\Delta\vec{r}$ and $\Delta\vec{p}$ are typically $\mathcal{O}(\Delta t)^2$. As any calculation of the evolution from time t_0 to t_f will involve a number $([t_f - t_0]/\Delta t)$ of time steps which grows inversely to Δt, the cumulative error can be expected to be $\mathcal{O}(\Delta t)$. In principle therefore we can approach exact results for a finite time evolution by taking smaller and smaller time steps, but in practise there are other considerations, such as computer time and roundoff errors, which argue strongly in favor of using more sophisticated numerical techniques, with errors of higher order in Δt. These can be found in any text on numerical methods.

Nonetheless, numerical solutions are often the only way to handle a real problem, and there has been extensive development of techniques for efficiently and accurately handling the problem, which is essentially one of solving a system of first order ordinary differential equations.

1.4.2 Phase Space Flows

As we just saw, Newton's equations for a system of particles can be cast in the form of a set of first order ordinary differential equations in time on phase space, with the motion in phase space described by the velocity field. This could be more generally discussed as a d'th order dynamical system, with a phase point representing the system in a d-dimensional phase space, moving with time t along the velocity field, sweeping out a path in phase space called the phase curve. The phase point $\vec{\eta}(t)$ is also called the state of the system at time t. Many qualitative features of the motion can be stated in terms of the phase curve.

Fixed Points

There may be points $\vec{\eta}_k$, known as **fixed points**, at which the velocity function vanishes, $\vec{V}(\vec{\eta}_k) = 0$. This is a point of equilibrium for the system, for if the system is at a fixed point at one moment, $\vec{\eta}(t_0) = \vec{\eta}_k$, it remains at that point. At other points, the system does not stay put, but there may be sets of states which flow into each other, such as the elliptical orbit for the undamped harmonic oscillator. These are called **invariant sets of states**. In a first order dynamical system[14], the fixed points divide the line into intervals which are invariant sets.

Even though a first-order system is smaller than any Newtonian system, it is worthwhile discussing briefly the phase flow there. We have been assuming the velocity function is a smooth function — generically its zeros will be first order, and near the fixed point η_0 we will have $V(\eta) \approx c(\eta - \eta_0)$. If the constant $c < 0$, $d\eta/dt$ will have the opposite sign from $\eta - \eta_0$, and the system will flow *towards* the fixed point,

[14]Note that this is not a one-dimensional Newtonian system, which is a two dimensional $\vec{\eta} = (x, p)$ dynamical system.

which is therefore called **stable**. On the other hand, if $c > 0$, the displacement $\eta - \eta_0$ will grow with time, and the fixed point is unstable. Of course there are other possibilities: if $V(\eta) = c\eta^2$, the fixed point $\eta = 0$ is stable from the left and unstable from the right. But this kind of situation is somewhat artificial, and such a system is **structually unstable**. What that means is that if the velocity field is perturbed by a small smooth variation $V(\eta) \to V(\eta) + \epsilon w(\eta)$, for some bounded smooth function w, the fixed point at $\eta = 0$ is likely to either disappear or split into two fixed points, whereas the fixed points discussed earlier will simply be shifted by order ϵ in position and will retain their stability or instability. Thus the simple zero in the velocity function is **structurally stable**. Note that structual stability is quite a different notion from stability of the fixed point.

In this discussion of stability in first order dynamical systems, we see that generically the stable fixed points occur where the velocity function decreases through zero, while the unstable points are where it increases through zero. Thus generically the fixed points will alternate in stability, dividing the phase line into open intervals which are each invariant sets of states, with the points in a given interval flowing either to the left or to the right, but never leaving the open interval. The state never reaches the stable fixed point because the time $t = \int d\eta / V(\eta) \approx (1/c) \int d\eta/(\eta - \eta_0)$ diverges. On the other hand, in the case $V(\eta) = c\eta^2$, a system starting at η_0 at $t = 0$ has a motion given by $\eta = (\eta_0^{-1} - ct)^{-1}$, which runs off to infinity as $t \to 1/\eta_0 c$. Thus the solution terminates at $t = 1/\eta_0 c$, and makes no sense thereafter. This form of solution is called **terminating motion**.

For higher order dynamical systems, the d equations $V_i(\vec{\eta}) = 0$ required for a fixed point will generically determine the d variables η_j, so the generic form of the velocity field near a fixed point η_0 is $V_i(\vec{\eta}) = \sum_j M_{ij}(\eta_j - \eta_{0j})$ with a nonsingular matrix M. The stability of the flow will be determined by this d-dimensional square matrix M. Generically the eigenvalue equation, a d'th order polynomial in λ, will have d distinct solutions. Because M is a real matrix, the eigenvalues must either be real or come in complex conjugate pairs. For the real case, whether the eigenvalue is positive or negative determines the instability or stability of the flow along the direction of the eigenvector. For a pair of complex conjugate eigenvalues $\lambda = u + iv$ and $\lambda^* = u - iv$,

with eigenvectors $\vec{e}$ and $\vec{e}^*$ respectively, we may describe the flow in the plane $\delta\vec{\eta} = \vec{\eta} - \vec{\eta}_0 = x(\vec{e} + \vec{e}^*) + iy(\vec{e} - \vec{e}^*)$, so

$$\begin{aligned} \dot{\vec{\eta}} &= M \cdot \delta\vec{\eta} = x(\lambda\vec{e} + \lambda^*\vec{e}^*) + iy(\lambda\vec{e} - \lambda^*\vec{e}^*) \\ &= (ux - vy)(\vec{e} + \vec{e}^*) + (vx + uy)(\vec{e} - \vec{e}^*) \end{aligned}$$

so

$$\begin{pmatrix} \dot{x} \\ \dot{y} \end{pmatrix} = \begin{pmatrix} u & -v \\ v & u \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix}, \qquad \text{or } \begin{cases} x &= Ae^{ut}\cos(vt + \phi) \\ y &= Ae^{ut}\sin(vt + \phi) \end{cases}.$$

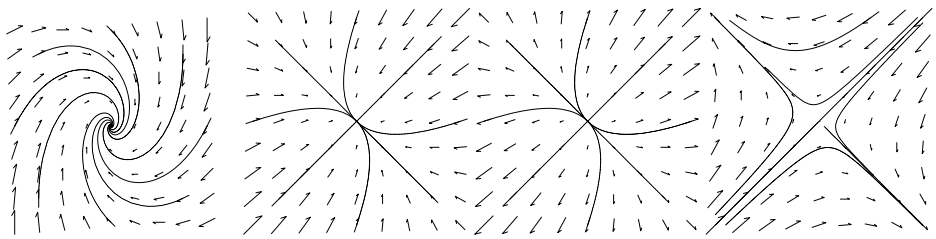
Thus we see that the motion spirals in towards the fixed point if u is negative, and spirals away from the fixed point if u is positive. Stability in these directions is determined by the sign of the real part of the eigenvalue.

In general, then, stability in each subspace around the fixed point $\vec{\eta}_0$ depends on the sign of the real part of the eigenvalue. If all the real parts are negative, the system will flow from anywhere in some neighborhood of $\vec{\eta}_0$ towards the fixed point, so $\lim_{t\to\infty} \vec{\eta}(t) = \vec{\eta}_0$ provided we start in that neighborhood. Then $\vec{\eta}_0$ is an **attractor** and is a **strongly stable** fixed point. On the other hand, if some of the eigenvalues have positive real parts, there are unstable directions. Starting from a generic point in any neighborhood of $\vec{\eta}_0$, the motion will eventually flow out along an unstable direction, and the fixed point is considered **unstable**, although there may be subspaces along which the flow may be into $\vec{\eta}_0$. An example is the line $x = y$ in the **hyperbolic fixed point** case shown in Figure 1.2.

Some examples of two dimensional flows in the neighborhood of a generic fixed point are shown in Figure 1.2. Note that none of these describe the fixed point of the undamped harmonic oscillator of Figure 1.1. We have discussed *generic* situations as if the velocity field were chosen arbitrarily from the set of all smooth vector functions, but in fact Newtonian mechanics imposes constraints on the velocity fields in many situations, in particular if there are conserved quantities.

Effect of conserved quantities on the flow

If the system has a conserved quantity $Q(q, p)$ which is a function on phase space only, and not of time, the flow in phase space is considerably changed. This is because the equations $Q(q, p) = K$ gives a set



$\dot{x} = -x + y,$	$\dot{x} = -3x - y,$	$\dot{x} = 3x + y,$	$\dot{x} = -x - 3y,$
$\dot{y} = -2x - y.$	$\dot{y} = -x - 3y.$	$\dot{y} = x + 3y.$	$\dot{y} = -3x - y.$
Strongly stable spiral point.	Strongly stable fixed point,	Unstable fixed point,	Hyperbolic fixed point,
$\lambda = -1 \pm \sqrt{2}i.$	$\lambda = -1, -2.$	$\lambda = 1, 2.$	$\lambda = -2, 1.$

Figure 1.2: Four generic fixed points for a second order dynamical system.

of subsurfaces or contours in phase space, and the system is confined to stay on whichever contour it is on initially. Unless this conserved quantity is a trivial function, *i.e.* constant, in the vicinity of a fixed point, it is not possible for all points to flow into the fixed point, and thus it is not strongly stable. In the terms of our generic discussion, the gradient of Q gives a direction orthogonal to the image of M, so there is a zero eigenvalue and we are not in the generic situation we discussed.

For the case of a single particle in a potential, the total energy $E = p^2/2m + U(\vec{r})$ is conserved, and so the motion of the system is confined to one surface of a given energy. As $\vec{p}/m$ is part of the velocity function, a fixed point must have $\vec{p} = 0$. The vanishing of the other half of the velocity field gives $\nabla U(\vec{r}_0) = 0$, which is the condition for a stationary point of the potential energy, and for the force to vanish. If this point is a maximum or a saddle of U, the motion along a descending path will be unstable. If the fixed point is a minimum of the potential, the region $E(\vec{r}, \vec{p}) < E(\vec{r}_0, 0) + \epsilon$, for

sufficiently small ϵ, gives a neighborhood around $\vec{\eta}_0 = (\vec{r}_0, 0)$ to which the motion is confined if it starts within this region. Such a fixed point is called **stable**[15], but it is not strongly stable, as the flow does not settle down to $\vec{\eta}_0$. This is the situation we saw for the undamped harmonic oscillator. For that situation $F = -kx$, so the potential energy may be taken to be

$$U(x) = \int_x^0 -kx \; dx = \frac{1}{2}kx^2,$$

and so the total energy $E = p^2/2m + \frac{1}{2}kx^2$ is conserved. The curves of constant E in phase space are ellipses, and each motion orbits the appropriate ellipse, as shown in Fig. 1.1 for the undamped oscillator. This contrasts to the case of the damped oscillator, for which there is no conserved energy, and for which the origin is a *strongly* stable fixed point.

[15] A fixed point is **stable** if it is in arbitrarity small neighborhoods, each with the property that if the system is in that neighborhood at one time, it remains in it at all later times.

As an example of a conservative system with both stable and unstable fixed points, consider a particle in one dimension with a cubic potential $U(x) = ax^2 - bx^3$, as shown in Fig. 1.3. There is a stable equilibrium at $x_s = 0$ and an unstable one at $x_u = 2a/3b$. Each has an associated fixed point in phase space, an **elliptic fixed point** $\eta_s = (x_s, 0)$ and a hyperbolic fixed point $\eta_u = (x_u, 0)$. The velocity field in phase space and several possible orbits are shown. Near the stable equilibrium, the trajectories are approximately ellipses, as they were for the harmonic oscillator, but for larger energies they begin to feel the asymmetry of the potential, and the orbits become egg-shaped.

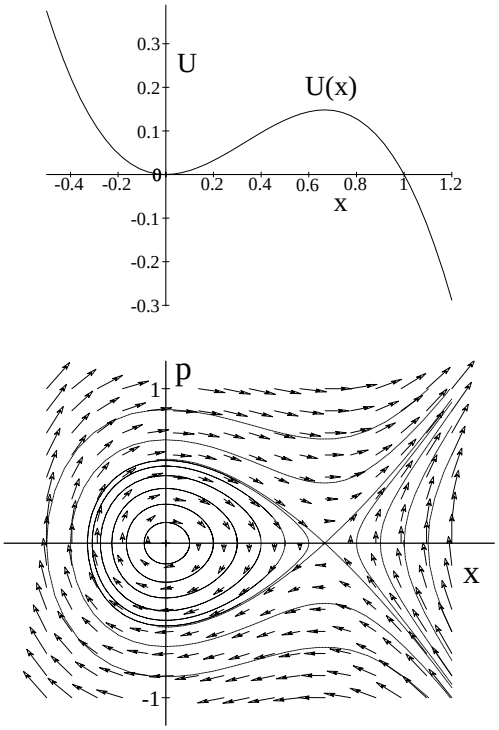


Figure 1.3. Motion in a cubic potential.

If the system has total energy precisely $U(x_u)$, the contour line crosses itself. This contour actually consists of three separate orbits. One starts at $t \to -\infty$ at $x = x_u$, completes one trip though the potential well, and returns as $t \to +\infty$ to $x = x_u$. The other two are orbits which go from $x = x_u$ to $x = \infty$, one incoming and one outgoing. For $E > U(x_u)$, all the orbits start and end at $x = +\infty$. Note that generically the orbits deform continuously as the energy varies, but at $E = U(x_u)$ this is not the case — the character of the orbit changes as E passes through $U(x_u)$. An orbit with this critical value of the energy is called a **seperatrix**, as it seperates regions in phase space where the orbits have different qualitative characteristics.

Quite generally hyperbolic fixed points are at the ends of seperatrices. In our case the contour $E = U(x_u)$ consists of four invariant sets

of states, one of which is the point η_u itself, and the other three are the orbits which are the disconnected pieces left of the contour after removing η_u.

Exercises

1.1 (a) Find the potential energy function $U(\vec{r})$ for a particle in the gravitational field of the Earth, for which the force law is $\vec{F}(\vec{r}) = -GM_E m\vec{r}/r^3$. (b) Find the escape velocity from the Earth, that is, the minimum velocity a particle near the surface can have for which it is possible that the particle will eventually coast to arbitrarily large distances without being acted upon by any force other than gravity. The Earth has a mass of 6.0×10^{24} kg and a radius of 6.4×10^6 m. Newton's gravitational constant is $6.67 \times 10^{-11}\mathrm{N} \cdot \mathrm{m}^2/\mathrm{kg}^2$.

1.2 In the discussion of a system of particles, it is important that the particles included in the system remain the same. There are some situations in which we wish to focus our attention on a set of particles which changes with time, such as a rocket ship which is emitting gas continuously. The equation of motion for such a problem may be derived by considering an infinitesimal time interval, $[t, t + \Delta t]$, and choosing the system to be the rocket with the fuel still in it at time t, so that at time $t + \Delta t$ the system consists of the rocket with its remaining fuel *and also* the small amount of fuel emitted during the infinitesimal time interval.
Let $M(t)$ be the mass of the rocket and remaining fuel at time t, assume that the fuel is emitted with velocity $\vec{u}$ with respect to the rocket, and call the velocity of the rocket $\vec{v}(t)$ in an inertial coordinate system. If the external force on the rocket is $\vec{F}(t)$ and the external force on the infinitesimal amount of exhaust is infinitesimal, the fact that $F(t)$ is the rate of change of the total momentum gives the equation of motion for the rocket.
(a) Show that this equation is

$$M\frac{d\vec{v}}{dt} = \vec{F}(t) + \vec{u}\frac{dM}{dt}.$$

(b) Suppose the rocket is in a constant gravitational field $\vec{F} = -Mg\hat{e}_z$ for the period during which it is burning fuel, and that it is fired straight up with constant exhaust velocity ($\vec{u} = -u\hat{e}_z$), starting from rest. Find $v(t)$ in terms of t and $M(t)$.
(c) Find the maximum fraction of the initial mass of the rocket which can escape the Earth's gravitational field if $u = 2000$m/s.

1.3 For a particle in two dimensions, we might use polar coordinates (r, θ) and use basis unit vectors $\hat{e}_r$ and $\hat{e}_\theta$ in the radial and tangent directions respectively to describe more general vectors. Because this pair of unit vectors differ from point to point, the $\hat{e}_r$ and $\hat{e}_\theta$ along the trajectory of a moving particle are themselves changing with time.
(a) Show that

$$\frac{d}{dt}\hat{e}_r = \dot{\theta}\hat{e}_\theta, \qquad \frac{d}{dt}\hat{e}_\theta = -\dot{\theta}\hat{e}_r.$$

(b) Thus show that the derivative of $\vec{r} = r\hat{e}_r$ is

$$\vec{v} = \dot{r}\hat{e}_r + r\dot{\theta}\hat{e}_\theta,$$

which verifies the discussion of Sec. (1.3.4).
(c) Show that the derivative of the velocity is

$$\vec{a} = \frac{d}{dt}\vec{v} = (\ddot{r} - r\dot{\theta}^2)\hat{e}_r + (r\ddot{\theta} + 2\dot{r}\dot{\theta})\hat{e}_\theta.$$

(d) Thus Newton's Law says for the radial and tangential components of the force are $F_r = \hat{e}_r \cdot F = m(\ddot{r} - r\dot{\theta}^2)$, $F_\theta = \hat{e}_\theta \cdot F = m(r\ddot{\theta} + 2\dot{r}\dot{\theta})$. Show that the generalized forces are $Q_r = F_r$ and $Q_\theta = rF_\theta$.

1.4 Analyze the errors in the integration of Newton's Laws in the simple Euler's approach described in section 1.4.1, where we approximated the change for x and p in each time interval Δt between t_i and t_{i+1} by $\dot{x}(t) \approx \dot{x}(t_i)$, $\dot{p}(t) \approx F(x(t_i), v(t_i))$. Assuming F to be differentiable, show that the error which accumulates in a finite time interval T is of order $(\Delta t)^1$.

1.5 Write a simple program to integrate the equation of the harmonic oscillator through one period of oscillation, using Euler's method with a step size Δt. Do this for several Δt, and see whether the error accumulated in one period meets the expectations of problem 1.4.

1.6 Describe the one dimensional phase space for the logistic equation $\dot{p} = bp - cp^2$, with $b > 0, c > 0$. Give the fixed points, the invariant sets of states, and describe the flow on each of the invariant sets.

1.7 Consider a pendulum consisting of a mass at the end of a massless rod of length L, the other end of which is fixed but free to rotate. Ignore one of the horizontal directions, and describe the dynamics in terms of the angle θ

between the rod and the downwards direction, without making a small angle approximation.
(a) Find the generalized force Q_θ and find the conserved quantity on phase space.
(b) Give a sketch of the velocity function, including all the regions of phase space. Show all fixed points, seperatrices, and describe all the invariant sets of states. [Note: the variable θ is defined only modulo 2π, so the phase space is the Cartesian product of an interval of length 2π in θ with the real line for p_θ. This can be plotted on a strip, with the understanding that the left and right edges are identified. To avoid having important points on the boundary, it would be well to plot this with $\theta \in [-\pi/2, 3\pi/2]$.

Chapter 2

Lagrange's and Hamilton's Equations

In this chapter, we consider two reformulations of Newtonian mechanics, the Lagrangian and the Hamiltonian formalism. The first is naturally associated with configuration space, extended by time, while the latter is the natural description for working in phase space.

Lagrange developed his approach in 1764 in a study of the libration of the moon, but it is best thought of as a general method of treating dynamics in terms of generalized coordinates for configuration space. It so transcends its origin that the Lagrangian is considered the fundamental object which describes a quantum field theory.

Hamilton's approach arose in 1835 in his unification of the language of optics and mechanics. It too had a usefulness far beyond its origin, and the Hamiltonian is now most familiar as the operator in quantum mechanics which determines the evolution in time of the wave function.

2.1 Lagrangian Mechanics

We begin by deriving Lagrange's equation as a simple change of coordinates in an unconstrained system, one which is evolving according to Newton's laws with force laws given by some potential. Lagrangian mechanics is also and especially useful in the presence of constraints, so we will then extend the formalism to this more general situation.

2.1.1 Derivation for unconstrained systems

For a collection of particles with conservative forces described by a potential, we have in inertial cartesian coordinates

$$m\ddot{x}_i = F_i.$$

The left hand side of this equation is determined by the kinetic energy function as the time derivative of the momentum $p_i = \partial T/\partial \dot{x}_i$, while the right hand side is a derivative of the potential energy, $-\partial U/\partial x_i$. As T is independent of x_i and U is independent of $\dot{x}_i$ in these coordinates, we can write both sides in terms of the **Lagrangian** $L = T - U$, which is then a function of both the coordinates and their velocities. Thus we have established

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{x}_i} - \frac{\partial L}{\partial x_i} = 0,$$

which, once we generalize it to arbitrary coordinates, will be known as Lagrange's equation. This particular combination of $T(\dot{\vec{r}})$ with $U(\vec{r})$ to get the more complicated $L(\vec{r}, \dot{\vec{r}})$ seems an artificial construction for the inertial cartesian coordinates, but it has the advantage of preserving the form of Lagrange's equations for any set of generalized coordinates.

As we did in section 1.3.3, we assume we have a set of generalized coordinates $\{q_j\}$ which parameterize all of coordinate space, so that each point may be described by the $\{q_j\}$ or by the $\{x_i\}$, $i, j \in [1, N]$, and thus each set may be thought of as a function of the other, and time:

$$q_j = q_j(x_1, ...x_N, t) \qquad x_i = x_i(q_1, ...q_N, t). \tag{2.1}$$

We may consider L as a function[1] of the generalized coordinates q_j and $\dot{q}_j$, and ask whether the same expression in these coordinates

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{q}_j} - \frac{\partial L}{\partial q_j}$$

[1]Of course we are not saying that $L(x, \dot{x}, t)$ is the same function of its coordinates as $L(q, \dot{q}, t)$, but rather that these are two functions which agree at the corresponding physical points. More precisely, we are defining a new function $\tilde{L}(q, \dot{q}, t) = L(x(q, t), \dot{x}(q, \dot{q}, t), t)$, but we are being physicists and neglecting the tilde. We are treating the Lagrangian here as a *scalar* under coordinate transformations, in the sense used in general relativity, that its value at a given physical point is unchanged by changing the coordinate system used to define that point.

also vanishes. The chain rule tells us

$$\frac{\partial L}{\partial \dot{x}_j} = \sum_k \frac{\partial L}{\partial q_k}\frac{\partial q_k}{\partial \dot{x}_j} + \sum_k \frac{\partial L}{\partial \dot{q}_k}\frac{\partial \dot{q}_k}{\partial \dot{x}_j}. \tag{2.2}$$

The first term vanishes because q_k depends only on the coordinates x_k and t, but not on the $\dot{x}_k$. From the inverse relation to (1.10),

$$\dot{q}_j = \sum_i \frac{\partial q_j}{\partial x_i}\dot{x}_i + \frac{\partial q_j}{\partial t}, \tag{2.3}$$

we have

$$\frac{\partial \dot{q}_j}{\partial \dot{x}_i} = \frac{\partial q_j}{\partial x_i}.$$

Using this in (2.2),

$$\frac{\partial L}{\partial \dot{x}_i} = \sum_j \frac{\partial L}{\partial \dot{q}_j}\frac{\partial q_j}{\partial x_i}. \tag{2.4}$$

Lagrange's equation involves the time derivative of this. Here what is meant is not a partial derivative $\partial/\partial t$, holding the point in configuration space fixed, but rather the derivative along the path which the system takes as it moves through configuration space. It is called the **stream derivative**, a name which comes from fluid mechanics, where it gives the rate at which some property defined throughout the fluid, $f(\vec{r}, t)$, changes for a fixed element of fluid as the fluid as a whole flows. We write it as a *total* derivative to indicate that we are following the motion rather than evaluating the rate of change at a fixed point in space, as the partial derivative does.

For any function $f(x, t)$ of extended configuration space, this total time derivative is

$$\frac{df}{dt} = \sum_j \frac{\partial f}{\partial x_j}\dot{x}_j + \frac{\partial f}{\partial t}. \tag{2.5}$$

Using Leibnitz' rule on (2.4) and using (2.5) in the second term, we find

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{x}_i} = \sum_j \left(\frac{d}{dt}\frac{\partial L}{\partial \dot{q}_j}\right)\frac{\partial q_j}{\partial x_i} + \sum_j \frac{\partial L}{\partial \dot{q}_j}\left(\sum_k \frac{\partial^2 q_j}{\partial x_i \partial x_k}\dot{x}_k + \frac{\partial^2 q_j}{\partial x_i \partial t}\right). \tag{2.6}$$

On the other hand, the chain rule also tells us

$$\frac{\partial L}{\partial x_i} = \sum_j \frac{\partial L}{\partial q_j}\frac{\partial q_j}{\partial x_i} + \sum_j \frac{\partial L}{\partial \dot{q}_j}\frac{\partial \dot{q}_j}{\partial x_i},$$

where the last term does not necessarily vanish, as $\dot{q}_j$ in general depends on both the coordinates and velocities. In fact, from 2.3,

$$\frac{\partial \dot{q}_j}{\partial x_i} = \sum_k \frac{\partial^2 q_j}{\partial x_i \partial x_k}\dot{x}_k + \frac{\partial^2 q_j}{\partial x_i \partial t},$$

so

$$\frac{\partial L}{\partial x_i} = \sum_j \frac{\partial L}{\partial q_j}\frac{\partial q_j}{\partial x_i} + \sum_j \frac{\partial L}{\partial \dot{q}_j}\left(\sum_k \frac{\partial^2 q_j}{\partial x_i \partial x_k}\dot{x}_k + \frac{\partial^2 q_j}{\partial x_i \partial t}\right). \tag{2.7}$$

Lagrange's equation in cartesian coordinates says (2.6) and (2.7) are equal, and in subtracting them the second terms cancel[2], so

$$0 \;=\; \sum_j \left(\frac{d}{dt}\frac{\partial L}{\partial \dot{q}_j} - \frac{\partial L}{\partial q_j}\right)\frac{\partial q_j}{\partial x_i}.$$

The matrix $\partial q_j/\partial x_i$ is nonsingular, as it has $\partial x_i/\partial q_j$ as its inverse, so we have derived Lagrange's Equation in generalized coordinates:

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{q}_j} - \frac{\partial L}{\partial q_j} = 0.$$

Thus we see that Lagrange's equations are form invariant under changes of the generalized coordinates used to describe the configuration of the system. It is primarily for this reason that this particular and peculiar combination of kinetic and potential energy is useful. Note that we implicity assume the Lagrangian itself transformed like a scalar, in that its value at a given physical point of configuration space is independent of the choice of generalized coordinates that describe the point. The change of coordinates itself (2.1) is called a **point transformation**.

[2]This is why we chose the particular combination we did for the Lagrangian, rather than $L = T - \alpha U$ for some $\alpha \neq 1$. Had we done so, Lagrange's equation in cartesian coordinates would have been $\alpha\ d(\partial L/\partial \dot{x}_j)/dt - \partial L/\partial x_j = 0$, and in the subtraction of (2.7) from $\alpha\times$(2.6), the terms proportional to $\partial L/\partial \dot{q}_i$ (without a time derivative) would not have cancelled.

2.1.2 Lagrangian for Constrained Systems

We now wish to generalize our discussion to include contraints. At the same time we will also consider possibly nonconservative forces. As we mentioned in section 1.3.2, we often have a system with internal forces whose effect is better understood than the forces themselves, with which we may not be concerned. We will assume the constraints are holonomic, expressible as k real functions $\Phi_\alpha(\vec{r}_1, ..., \vec{r}_n, t) = 0$, which are somehow enforced by constraint forces $\vec{F}_i^C$ on the particle i. There may also be other forces, which we will call F_i^D and will treat as having a dynamical effect. These are given by known functions of the configuration and time, possibly but not necessarily in terms of a potential.

This distinction will seem artificial without examples, so it would be well to keep these two in mind. In each of these cases the full configuration space is $\mathbb{R}^3$, but the constraints restrict the motion to an allowed subspace of extended configuration space.

1. In section 1.3.2 we discussed a mass on a light rigid rod, the other end of which is fixed at the origin. Thus the mass is constrained to have $|\vec{r}| = L$, and the allowed subspace of configuration space is the surface of a sphere, independent of time. The rod exerts the constraint force to avoid compression or expansion. The natural assumption to make is that the force is in the radial direction, and therefore has no component in the direction of allowed motions, the tangential directions. That is, for all allowed displacements, $\delta\vec{r}$, we have $\vec{F}^C \cdot \delta\vec{r} = 0$, and the constraint force does no work.

2. Consider a bead free to slide without friction on the spoke of a rotating bicycle wheel[3], rotating about a fixed axis at fixed angular velocity ω. That is, for the polar angle θ of inertial coordinates, $\Phi := \theta - \omega t = 0$ is a constraint[4], but the r coordinate is unconstrained. Here the allowed subspace is not time independent, but is a helical sort of structure in extended configuration space. We expect the force exerted by the spoke on the bead to be in the $\hat{e}_\theta$

[3]Unlike a real bicycle wheel, we are assuming here that the spoke is directly along a radius of the circle, pointing directly to the axle.

[4]There is also a constraint $z = 0$.

direction. This is again perpendicular to any **virtual displacement**, by which we mean an allowed change in configuration *at a fixed time*. It is important to distinguish this virtual displacement from a small segment of the trajectory of the particle. In this case a virtual displacement is a change in r without a change in θ, and is perpendicular to $\hat{e}_\theta$. So again, we have the "net virtual work" of the constraint forces is zero. It is important to note that this does not mean that the net real work is zero. In a small time interval, the displacement $\Delta\vec{r}$ includes a component $r\omega\Delta t$ in the tangential direction, and the force of constraint does do work!

We will assume that the constraint forces in general satisfy this restriction that no net *virtual* work is done by the forces of constraint for any possible virtual displacement. Newton's law tells us that $\dot{\vec{p}}_i = F_i = F_i^C + F_i^D$. We can multiply by an arbitrary virtual displacement

$$\sum_i \left(\vec{F}_i^D - \dot{\vec{p}}_i\right) \cdot \delta\vec{r}_i = -\sum_i \vec{F}_i^C \cdot \delta\vec{r}_i = 0,$$

where the first equality would be true even if $\delta\vec{r}_i$ did not satisfy the constraints, but the second requires $\delta\vec{r}_i$ to be an allowed virtual displacement. Thus

$$\sum_i \left(\vec{F}_i^D - \dot{\vec{p}}_i\right) \cdot \delta\vec{r}_i = 0, \tag{2.8}$$

which is known as **D'Alembert's Principle**. This gives an equation which determines the motion on the constrained subspace and does not involve the unspecified forces of constraint F^C. We drop the superscript ^{D} from now on.

Suppose we know generalized coordinates $q_1, \ldots, q_N$ which parameterize the constrained subspace, which means $\vec{r}_i = \vec{r}_i(q_1, \ldots, q_N, t)$, for $i = 1, \ldots, n$, are known functions and the N q's are independent. There are $N = 3n - k$ of these independent coordinates, where k is the number of holonomic constraints. Then $\partial\vec{r}_i/\partial q_j$ is no longer an invertable, or even square, matrix, but we still have

$$\Delta\vec{r}_i = \sum_j \frac{\partial\vec{r}_i}{\partial q_j}\Delta q_j + \frac{\partial\vec{r}_i}{\partial t}\Delta t.$$

For the velocity of the particle, divide this by Δt, giving

$$\vec{v}_i = \sum_j \frac{\partial \vec{r}_i}{\partial q_j}\dot{q}_j + \frac{\partial \vec{r}_i}{\partial t}, \tag{2.9}$$

but for a *virtual* displacement $\Delta t = 0$ we have

$$\delta\vec{r}_i = \sum_j \frac{\partial \vec{r}_i}{\partial q_j}\delta q_j.$$

Differentiating (2.9) we note that,

$$\frac{\partial \vec{v}_i}{\partial \dot{q}_j} = \frac{\partial \vec{r}_i}{\partial q_j}, \tag{2.10}$$

and also

$$\frac{\partial \vec{v}_i}{\partial q_j} = \sum_k \frac{\partial^2 \vec{r}_i}{\partial q_j \partial q_k}\dot{q}_k + \frac{\partial^2 \vec{r}_i}{\partial q_j \partial t} = \frac{d}{dt}\frac{\partial \vec{r}_i}{\partial q_j}, \tag{2.11}$$

where the last equality comes from applying (2.5), with coordinates q_j rather than x_j, to $f = \partial\vec{r}_i/\partial q_j$. The first term in the equation (2.8) stating D'Alembert's principle is

$$\sum_i \vec{F}_i \cdot \delta\vec{r}_i = \sum_j \sum_i \vec{F}_i \cdot \frac{\partial \vec{r}_i}{\partial q_j}\delta q_j = \sum_j Q_j \cdot \delta q_j.$$

The generalized force Q_j has the same form as in the unconstrained case, as given by (1.9), but there are only as many of them as there are *unconstrained* degrees of freedom.

The second term involves

$$\begin{aligned}
\sum_i \dot{\vec{p}}_i \cdot \delta\vec{r}_i &= \sum_i \frac{dp_i}{dt}\frac{\partial \vec{r}_i}{\partial q_j}\delta q_j \\
&= \sum_j \frac{d}{dt}\left(\sum_i \vec{p}_i \cdot \frac{\partial \vec{r}_i}{\partial q_j}\right)\delta q_j - \sum_{ij} p_i \cdot \left(\frac{d}{dt}\frac{\partial \vec{r}_i}{\partial q_j}\right)\delta q_j \\
&= \sum_j \frac{d}{dt}\left(\sum_i \vec{p}_i \cdot \frac{\partial \vec{v}_i}{\partial \dot{q}_j}\right)\delta q_j - \sum_{ij} p_i \cdot \frac{\partial \vec{v}_i}{\partial q_j}\delta q_j \\
&= \sum_j \left[\frac{d}{dt}\sum_i m_i \vec{v}_i \cdot \frac{\partial \vec{v}_i}{\partial \dot{q}_j} - \sum_i m_i v_i \cdot \frac{\partial \vec{v}_i}{\partial q_j}\right]\delta q_j \\
&= \sum_j \left[\frac{d}{dt}\frac{\partial T}{\partial \dot{q}_j} - \frac{\partial T}{\partial q_j}\right]\delta q_j,
\end{aligned}$$

where we used (2.10) and (2.11) to get the third line. Plugging in the expressions we have found for the two terms in D'Alembert's Principle,

$$\sum_j \left[\frac{d}{dt}\frac{\partial T}{\partial \dot{q}_j} - \frac{\partial T}{\partial q_j} - Q_j \right] \delta q_j = 0.$$

We assumed we had a holonomic system and the q's were all independent, so this equation holds for arbitrary virtual displacements δq_j, and therefore

$$\frac{d}{dt}\frac{\partial T}{\partial \dot{q}_j} - \frac{\partial T}{\partial q_j} - Q_j = 0. \tag{2.12}$$

Now let us restrict ourselves to forces given by a potential, with $\vec{F}_i = -\vec{\nabla}_i U(\{\vec{r}\}, t)$, or

$$Q_j = -\sum_i \frac{\partial \vec{r}_i}{\partial q_j} \cdot \vec{\nabla}_i U = -\left. \frac{\partial \tilde{U}(\{q\}, t)}{\partial q_j} \right|_t .$$

Notice that Q_j depends only on the value of U on the constrained surface. Also, U is independent of the $\dot{q}_i$'s, so

$$\frac{d}{dt}\frac{\partial T}{\partial \dot{q}_j} - \frac{\partial T}{\partial q_j} + \frac{\partial U}{\partial q_j} = 0 = \frac{d}{dt}\frac{\partial (T-U)}{\partial \dot{q}_j} - \frac{\partial (T-U)}{\partial q_j},$$

or

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{q}_j} - \frac{\partial L}{\partial q_j} = 0. \tag{2.13}$$

This is Lagrange's equation, which we have now derived in the more general context of constrained systems.

Some examples of the use of Lagrangians

Atwood's machine consists of two blocks of mass m_1 and m_2 attached by an inextensible cord which suspends them from a pulley of moment of inertia I with frictionless bearings. The kinetic energy is

$$\begin{aligned} T &= \frac{1}{2} m_1 \dot{x}^2 + \frac{1}{2} m_2 \dot{x}^2 + \frac{1}{2} I \omega^2 \\ U &= m_1 g x + m_2 g (K - x) = (m_1 - m_2) g x + \text{const} \end{aligned}$$

where we have used the fact that the sum of the heights of the masses is a constant K. We assume the cord does not slip on the pulley, so the angular velocity of the pulley is $\omega = \dot{x}/r$, and

$$L = \frac{1}{2}(m_1 + m_2 + I/r^2)\dot{x}^2 + (m_2 - m_1)gx,$$

and Lagrange's equation gives

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{x}} - \frac{\partial L}{\partial x} = 0 = (m_1 + m_2 + I/r^2)\ddot{x} - (m_2 - m_1)g.$$

Notice that we set up our system in terms of only one degree of freedom, the height of the first mass. This one degree of freedom parameterizes the line which is the allowed subspace of the unconstrained configuration space, a three dimensional space which also has directions corresponding to the angle of the pulley and the height of the second mass. The constraints restrict these three variables because the string has a fixed length and does not slip on the pulley. Note that this formalism has permitted us to solve the problem without solving for the forces of constraint, which in this case are the tensions in the cord on either side of the pulley.

As a second example, reconsider the bead on the spoke of a rotating bicycle wheel. In section (1.3.4) we saw that the kinetic energy is $T = \frac{1}{2}m\dot{r}^2 + \frac{1}{2}mr^2\omega^2$. If there are no forces other than the constraint forces, $U(r, \theta) \equiv 0$, and the Lagrangian is

$$L = \frac{1}{2}m\dot{r}^2 + \frac{1}{2}mr^2\omega^2.$$

The equation of motion for the one degree of freedom is easy enough:

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{r}} = m\ddot{r} = \frac{\partial L}{\partial r} = mr\omega^2,$$

which looks like a harmonic oscillator with a negative spring constant, so the solution is a real exponential instead of oscillating,

$$r(t) = Ae^{-\omega t} + Be^{\omega t}.$$

The velocity-independent term in T acts just like a potential would, and can in fact be considered the potential for the centrifugal force.

But we see that the total energy T is not conserved but blows up as $t \to \infty$, $T \sim mB^2\omega^2 e^{2\omega t}$. This is because the force of constraint, while it does no *virtual* work, does do real work.

Finally, let us consider the mass on the end of the gimballed rod. The allowed subspace is the surface of a sphere, which can be parameterized by an azimuthal angle ϕ and the polar angle with the upwards direction, θ, in terms of which

$$z = \ell\cos\theta, \quad x = \ell\sin\theta\cos\phi, \quad y = \ell\sin\theta\sin\phi,$$

and $T = \frac{1}{2}m\ell^2(\dot\theta^2 + \sin^2\theta\dot\phi^2)$. With an arbitrary potential $U(\theta,\phi)$, the Lagrangian becomes

$$L = \frac{1}{2}m\ell^2(\dot\theta^2 + \sin^2\theta\dot\phi^2) - U(\theta,\phi).$$

From the two independent variables θ, ϕ there are two Lagrange equations of motion,

$$m\ell^2\ddot\theta = -\frac{\partial U}{\partial\theta} + \frac{1}{2}\sin(2\theta)\dot\phi^2, \tag{2.14}$$

$$\frac{d}{dt}\left(m\ell^2\sin^2\theta\dot\phi\right) = -\frac{\partial U}{\partial\phi}. \tag{2.15}$$

Notice that this is a dynamical system with two coordinates, similar to ordinary mechanics in two dimensions, except that the mass matrix, while diagonal, is coordinate dependent, and the space on which motion occurs is not an infinite flat plane, but a curved two dimensional surface, that of a sphere. These two distinctions are connected—the coordinates enter the mass matrix because it is impossible to describe a curved space with unconstrained cartesian coordinates.

2.1.3 Hamilton's Principle

The configuration of a system at any moment is specified by the value of the generalized coordinates $q_j(t)$, and the space coordinatized by these $q_1, \ldots, q_N$ is the **configuration space**. The time evolution of the system is given by the trajectory, or motion of the point in configuration space as a function of time, which can be specified by the *functions* $q_i(t)$.

One can imagine the system taking many paths, whether they obey Newton's Laws or not. We consider only paths for which the $q_i(t)$ are differentiable. Along any such path, we define the **action** as

$$I = \int_{t_1}^{t_2} L(q(t), \dot{q}(t), t)dt. \tag{2.16}$$

The action depends on the starting and ending points $q(t_1)$ and $q(t_2)$, but beyond that, the value of the action depends on the path, unlike the work done by a conservative force on a point moving in ordinary space. In fact, it is exactly this dependence on the path which makes this concept useful — Hamilton's principle states that the actual motion of the particle from $q(t_1) = q_i$ to $q(t_2) = q_f$ is along a path $q(t)$ for which the action is stationary. That means that for any small deviation of the path from the actual one, keeping the initial and final configurations fixed, the variation of the action vanishes to first order in the deviation.

To find out where a differentiable function of one variable has a stationary point, we differentiate and solve the equation found by setting the derivative to zero. If we have a differentiable function f of several variables x_i, the first-order variation of the function is $\Delta f = \sum_i (x_i - x_{0i})\, \partial f/\partial x_i|_{x_0}$, so unless $\partial f/\partial x_i|_{x_0} = 0$ for all i, there is some variation of the $\{x_i\}$ which causes a first order variation of f, and then x_0 is not a stationary point.

But our action is a **functional**, a function of functions, which represent an infinite number of variables, even for a path in only one dimension. Intuitively, at each time $q(t)$ is a separate variable, though varying q at only one point makes $\dot{q}$ hard to interpret. A rigorous mathematician might want to describe the path $q(t)$ on $t \in [0, 1]$ in terms of Fourier series, for which $q(t) = q_0 + q_1 t + \sum_{n=1} a_n \sin(n\pi t)$. Then the functional $I(f)$ given by

$$I = \int f(q(t), \dot{q}(t), t)dt$$

becomes a function of the infinitely many variables $q_0, q_1, a_1, \ldots$. The endpoints fix q_0 and q_1, but the stationary condition gives an infinite number of equations $\partial I/\partial a_n = 0$.

It is not really necessary to be so rigorous, however. Under a change $q(t) \to q(t) + \delta q(t)$, the derivative will vary by $\delta\dot{q} = d\,\delta q(t)/dt$, and the

functional I will vary by

$$\begin{aligned}\delta I &= \int \left(\frac{\partial f}{\partial q}\delta q + \frac{\partial f}{\partial \dot{q}}\delta \dot{q} \right) dt \\ &= \frac{\partial f}{\partial \dot{q}}\delta q \Big|_i^f + \int \left[\frac{\partial f}{\partial q} - \frac{d}{dt}\frac{\partial f}{\partial \dot{q}} \right] \delta q dt,\end{aligned}$$

where we integrated the second term by parts. The boundary terms each have a factor of δq at the initial or final point, which vanish because Hamilton tells us to hold the q_i and q_f fixed, and therefore the functional is stationary if and only if

$$\frac{\partial f}{\partial q} - \frac{d}{dt}\frac{\partial f}{\partial \dot{q}} = 0 \quad \text{for } t \in (t_i, t_f) \tag{2.17}$$

We see that if f is the Lagrangian, we get exactly Lagrange's equation. The above derivation is essentially unaltered if we have many degrees of freedom q_i instead of just one.

2.1.4 Examples of functional variation

In this section we will work through some examples of functional variations both in the context of the action and for other examples not directly related to mechanics.

The falling particle

As a first example of functional variation, consider a particle thrown up in a uniform gravitional field at $t = 0$, which lands at the same spot at $t = T$. The Lagrangian is $L = \frac{1}{2}m(\dot{x}^2 + \dot{y}^2 + \dot{z}^2) - mgz$, and the boundary conditions are $x(t) = y(t) = z(t) = 0$ at $t = 0$ and $t = T$. Elementary mechanics tells us the solution to this problem is $x(t) = y(t) \equiv 0$, $z(t) = v_0 t - \frac{1}{2}gt^2$ with $v_0 = \frac{1}{2}gT$. Let us evaluate the action for any other path, writing $z(t)$ in terms of its deviation from the suspected solution,

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

We make no assumptions about this path other than that it is differentiable and meets the boundary conditions $x = y = \Delta z = 0$ at $t = 0$ and at $t = T$. The action is

$$\begin{aligned} I &= \int_0^T \left\{ \frac{1}{2} m \left[\dot{x}^2 + \dot{y}^2 + \left(\frac{d\Delta z}{dt} \right)^2 + g(T-2t) \frac{d\Delta z}{dt} + \frac{1}{4} g^2 (T-2t)^2 \right] \right. \\ &\qquad \left. - mg\Delta z - \frac{1}{2} mg^2 t(T-t) \right\} dt. \end{aligned}$$

The fourth term can be integrated by parts,

$$\int_0^T \frac{1}{2} mg(T-2t) \frac{d\Delta z}{dt}\, dt = \frac{1}{2} mg(T-2t)\Delta z \Big|_0^T + \int_0^T mg\Delta z(t)\, dt.$$

The boundary term vanishes because $\Delta z = 0$ where it is evaluated, and the other term cancels the sixth term in I, so

$$\begin{aligned} I &= \int_0^T \frac{1}{2} mg^2 \left[\frac{1}{4} (T-2t)^2 - t(T-t) \right] dt \\ &\qquad + \int_0^T \frac{1}{2} m \left[\dot{x}^2 + \dot{y}^2 + \left(\frac{d\Delta z}{dt} \right)^2 \right]. \end{aligned}$$

The first integral is independent of the path, so the minimum action requires the second integral to be as small as possible. But it is an integral of a non-negative quantity, so its minimum is zero, requiring $\dot{x} = \dot{y} = d\Delta z/dt = 0$. As $x = y = \Delta z = 0$ at $t = 0$, this tells us $x = y = \Delta z = 0$ at all times, and the path which minimizes the action is the one we expect from elementary mechanics.

Is the shortest path a straight line?

The calculus of variations occurs in other contexts, some of which are more intuitive. The classic example is to find the shortest path between two points in the plane. The length ℓ of a path $y(x)$ from (x_1, y_1) to

(x_2, y_2) is given[5] by

$$\ell = \int_{x_1}^{x_2} ds = \int_{x_1}^{x_2} \sqrt{1 + \left(\frac{dy}{dx}\right)^2}\, dx.$$

We see that length ℓ is playing the role of the action, and x is playing the role of t. Using $\dot{y}$ to represent dy/dx, we have the integrand $f(y, \dot{y}, x) = \sqrt{1 + \dot{y}^2}$, and $\partial f/\partial y = 0$, so Eq. 2.17 gives

$$\frac{d}{dx}\frac{\partial f}{\partial \dot{y}} = \frac{d}{dx}\frac{\dot{y}}{\sqrt{1 + \dot{y}^2}} = 0, \quad \text{so } \dot{y} = \text{const.}$$

and the path is a straight line.

2.1.5 Conserved Quantities

Ignorable Coordinates

If the Lagrangian does not depend on one coordinate, say q_k, then we say it is an **ignorable coordinate**. Of course, we still want to solve for it, as its derivative may still enter the Lagrangian and effect the evolution of other coordinates. By Lagrange's equation

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{q}_k} = \frac{\partial L}{\partial q_k} = 0,$$

so if in general we define

$$P_k := \frac{\partial L}{\partial \dot{q}_k},$$

as the **generalized momentum**, then in the case that L is independent of q_k, P_k is conserved, $dP_k/dt = 0$.

Linear Momentum As a very elementary example, consider a particle under a force given by a potential which depends only on y and z, but not x. Then

$$L = \frac{1}{2}m\left(\dot{x}^2 + \dot{y}^2 + \dot{z}^2\right) - U(y, z)$$

[5]Here we are assuming the path is monotone in x, without moving somewhere to the left and somewhere to the right. To prove that the straight line is shorter than other paths which might not obey this restriction, do Exercise 2.2.

is independent of x, x is an ignorable coordinate and

$$P_x = \frac{\partial L}{\partial \dot{x}} = m\dot{x}$$

is conserved. This is no surprize, of course, because the force is $F = -\nabla U$ and $F_x = -\partial U/\partial x = 0$.

Note that, using the definition of the generalized momenta

$$P_k = \frac{\partial L}{\partial \dot{q}_k},$$

Lagrange's equation can be written as

$$\frac{d}{dt}P_k = \frac{\partial L}{\partial q_k} = \frac{\partial T}{\partial q_k} - \frac{\partial U}{\partial q_k}.$$

Only the last term enters the definition of the generalized force, so if the kinetic energy depends on the coordinates, as will often be the case, it is not true that $dP_k/dt = Q_k$. In that sense we might say that the generalized momentum and the generalized force *have not been defined consistently.*

Angular Momentum As a second example of a system with an ignorable coordinate, consider an axially symmetric system described with inertial polar coordinates (r, θ, z), with z along the symmetry axis. Extending the form of the kinetic energy we found in sec (1.3.4) to include the z coordinate, we have $T = \frac{1}{2}m\dot{r}^2 + \frac{1}{2}mr^2\dot{\theta}^2 + \frac{1}{2}m\dot{z}^2$. The potential is independent of θ, because otherwise the system would not be symmetric about the z-axis, so the Lagrangian

$$L = \frac{1}{2}m\dot{r}^2 + \frac{1}{2}mr^2\dot{\theta}^2 + \frac{1}{2}m\dot{z}^2 - U(r, z)$$

does not depend on θ, which is therefore an ignorable coordinate, and

$$P_\theta := \frac{\partial L}{\partial \dot{\theta}} = mr^2\dot{\theta} = \text{constant}.$$

We see that the conserved momentum P_θ is in fact the z-component of the angular momentum, and is conserved because the axially symmetric potential can exert no torque in the z-direction:

$$\tau_z = -\left(\vec{r} \times \vec{\nabla} U\right)_z = -r\left(\vec{\nabla} U\right)_\theta = -r^2\frac{\partial U}{\partial \theta} = 0.$$

Finally, consider a particle in a spherically symmetric potential in spherical coordinates. In section (3.1.2) we will show that the kinetic energy in spherical coordinates is $T = \frac{1}{2}m\dot{r}^2 + \frac{1}{2}mr^2\dot{\theta}^2 + \frac{1}{2}mr^2\sin^2\theta\dot{\phi}^2$, so the Lagrangian with a spherically symmetric potential is

$$L = \frac{1}{2}m\dot{r}^2 + \frac{1}{2}mr^2\dot{\theta}^2 + \frac{1}{2}mr^2\sin^2\theta\dot{\phi}^2 - U(r).$$

Again, ϕ is an ignorable coordinate and the conjugate momentum P_ϕ is conserved. Note, however, that even though the potential is independent of θ as well, θ does appear undifferentiated in the Lagrangian, and it is *not* an ignorable coordinate, nor is P_θ conserved[6].

Energy Conservation

We may ask what happens to the Lagrangian along the path of the motion.

$$\frac{dL}{dt} = \sum_i \frac{\partial L}{\partial q_i}\frac{dq_i}{dt} + \sum_i \frac{\partial L}{\partial \dot{q}_i}\frac{d\dot{q}_i}{dt} + \frac{\partial L}{\partial t}$$

In the first term the first factor is

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{q}_i}$$

by the equations of motion, so

$$\frac{dL}{dt} = \frac{d}{dt}\left(\sum_i \frac{\partial L}{\partial \dot{q}_i}\dot{q}_i\right) + \frac{\partial L}{\partial t}.$$

We expect energy conservation when the potential is time invariant and there is not time dependence in the constraints, *i.e.* when $\partial L/\partial t = 0$, so we rewrite this in terms of

$$H(q, \dot{q}, t) = \sum_i \dot{q}_i \frac{\partial L}{\partial \dot{q}_i} - L = \sum_i \dot{q}_i P_i - L$$

[6]It seems curious that we are finding straightforwardly one of the components of the conserved momentum, but not the other two, L_y and L_x, which are also conserved. The fact that not all of these emerge as conjugates to ignorable coordinates is related to the fact that the components of the angular momentum do not commute in quantum mechanics. This will be discussed further in section (6.6.1).

Then for the actual motion of the system,

$$\frac{dH}{dt} = -\frac{\partial L}{\partial t}.$$

If $\partial L/\partial t = 0$, H is conserved.

H is essentially the Hamiltonian, although strictly speaking that name is reserved for the function $H(q, p, t)$ on extended phase space rather than the function with arguments $(q, \dot{q}, t)$. What is H physically? In the case of Newtonian mechanics with a potential function, L is a quadratic function of the velocities $\dot{q}_i$. If we write the Lagrangian $L = L_2 + L_1 + L_0$ as a sum of pieces purely quadratic, purely linear, and independent of the velocities respectively, then

$$\sum_i \dot{q}_i \frac{\partial}{\partial \dot{q}_i}$$

is an operator which multiplies each term by its order in velocities,

$$\sum_i \dot{q}_i \frac{\partial L_i}{\partial \dot{q}_i} = iL_i, \qquad \sum_i \dot{q}_i \frac{\partial L}{\partial \dot{q}_i} = 2L_2 + L_1,$$

and

$$H = L_2 - L_0.$$

For a system of particles described by their cartesian coordinates, L_2 is just the kinetic energy T, while L_0 is the negative of the potential energy $L_0 = -U$, so $H = T + U$ is the ordinary energy. As we shall see later, however, there are constrained systems in which the Hamiltonian is conserved but is not the ordinary energy.

2.1.6 Hamilton's Equations

We have written the Lagrangian as a function of q_i, $\dot{q}_i$, and t, so it is a function of $N + N + 1$ variables. For a free particle we can write the kinetic energy either as $\frac{1}{2}m\dot{x}^2$ or as $p^2/2m$. More generally, we can[7] reexpress the dynamics in terms of the $2N + 1$ variables q_k, P_k, and t.

[7]In field theory there arise situations in which the set of functions $P_k(q_i, \dot{q}_i)$ cannot be inverted to give functions $\dot{q}_i = \dot{q}_i(q_j, P_j)$. This gives rise to local gauge invariance, and will be discussed in Chapter 8, but until then we will assume that the phase space (q, p), or cotangent bundle, is equivalent to the tangent bundle, *i.e.* the space of $(q, \dot{q})$.

The motion of the system sweeps out a path in the space $(q, \dot{q}, t)$ or a path in (q, P, t). Along this line, the variation of L is

$$\begin{aligned} dL &= \sum_k \left(\frac{\partial L}{\partial \dot{q}_k} d\dot{q}_k + \frac{\partial L}{\partial q_k} dq_k \right) + \frac{\partial L}{\partial t} dt \\ &= \sum_k \left(P_k d\dot{q}_k + \dot{P}_k dq_k \right) + \frac{\partial L}{\partial t} dt \end{aligned}$$

where for the first term we used the definition of the generalized momentum and in the second we have used the equations of motion $\dot{P}_k = \partial L/\partial q_k$. Then examining the change in the Hamiltonian $H = \sum_k P_k \dot{q}_k - L$ along this actual motion,

$$\begin{aligned} dH &= \sum_k \left(P_k d\dot{q}_k + \dot{q}_k dP_k \right) - dL \\ &= \sum_k \left(\dot{q}_k dP_k - \dot{P}_k dq_k \right) - \frac{\partial L}{\partial t} dt. \end{aligned}$$

If we think of $\dot{q}_k$ and H as functions of q and P, and think of H as a function of q, P, and t, we see that the physical motion obeys

$$\dot{q}_k = \left. \frac{\partial H}{\partial P_k} \right|_{q,t}, \qquad \dot{P}_k = - \left. \frac{\partial H}{\partial q_k} \right|_{P,t}, \qquad \left. \frac{\partial H}{\partial t} \right|_{q,P} = - \left. \frac{\partial L}{\partial t} \right|_{q,\dot{q}}$$

The first two constitute **Hamilton's equations of motion**, which are first order equations for the motion of the point representing the system in phase space.

Let's work out a simple example, the one dimensional harmonic oscillator. Here the kinetic energy is $T = \frac{1}{2} m \dot{x}^2$, the potential energy is $U = \frac{1}{2} k x^2$, so $L = \frac{1}{2} m \dot{x}^2 - \frac{1}{2} k x^2$, the only generalized momentum is $P = \partial L/\partial \dot{x} = m\dot{x}$, and the Hamiltonian is $H = P\dot{x} - L = P^2/m - (P^2/2m - \frac{1}{2} k x^2) = P^2/2m + \frac{1}{2} k x^2$. Note this is just the *sum* of the kinetic and potential energies, or the total energy.

Hamilton's equations give

$$\dot{x} = \left. \frac{\partial H}{\partial P} \right|_x = \frac{P}{m}, \qquad \dot{P} = - \left. \frac{\partial H}{\partial x} \right|_P = -kx = F.$$

These two equations verify the usual connection of the momentum and velocity and give Newton's second law.

The identification of H with the total energy is more general than our particular example. If T is purely quadratic in velocities, we can write $T = \frac{1}{2}\sum_{ij} M_{ij}\dot{q}_i\dot{q}_j$ in terms of a symmetric **mass matrix** M_{ij}. If in addition U is independent of velocities,

$$\begin{aligned} L &= \frac{1}{2}\sum_{ij} M_{ij}\dot{q}_i\dot{q}_j - U(q) \\ P_k &= \frac{\partial L}{\partial \dot{q}_k} = \sum_i M_{ki}\dot{q}_i \end{aligned}$$

which as a matrix equation in a n-dimensional space is $P = M \cdot \dot{q}$. Assuming M is invertible,[8] we also have $\dot{q} = M^{-1} \cdot P$, so

$$\begin{aligned} H &= P^T \cdot \dot{q} - L \\ &= P^T \cdot M^{-1} \cdot P - \left(\frac{1}{2}\dot{q}^T \cdot M \cdot \dot{q} - U(q)\right) \\ &= P^T \cdot M^{-1} \cdot P - \frac{1}{2}P^T \cdot M^{-1} \cdot M \cdot M^{-1} \cdot P + U(q) \\ &= \frac{1}{2}P^T \cdot M^{-1} \cdot P + U(q) = T + U \end{aligned}$$

so we see that the Hamiltonian is indeed the total energy under these circumstances.

2.1.7 Velocity-dependent forces

We have concentrated thus far on Newtonian mechanics with a potential given as a function of coordinates only. As the potential is a piece of the Lagrangian, which may depend on velocities as well, we should also entertain the possibility of velocity-dependent potentials. Only by

[8] If M were not invertible, there would be a linear combination of velocities which does not affect the Lagrangian. The degree of freedom corresponding to this combination would have a Lagrange equation without time derivatives, so it would be a constraint equation rather than an equation of motion. But we are assuming that the q's are a set of independent generalized coordinates that have already been pruned of all constraints.

considering such a potential can we possibly find velocity-dependent forces, and one of the most important force laws in physics is of that form. This is the Lorentz force[9] on a particle of charge q in the presence of electromagnetic fields $\vec{E}(\vec{r},t)$ and $\vec{B}(\vec{r},t)$,

$$\vec{F} = q\left(\vec{E} + \frac{\vec{v}}{c} \times \vec{B}\right). \tag{2.18}$$

If the motion of a charged particle is described by Lagrangian mechanics with a potential $U(\vec{r},\vec{v},t)$, Lagrange's equation says

$$0 = \frac{d}{dt}\frac{\partial L}{\partial v_i} - \frac{\partial L}{\partial r_i} = m\ddot{r}_i - \frac{d}{dt}\frac{\partial U}{\partial v_i} + \frac{\partial U}{\partial r_i}, \qquad \text{so } F_i = \frac{d}{dt}\frac{\partial U}{\partial v_i} - \frac{\partial U}{\partial r_i}.$$

We want a force linear in $\vec{v}$ and proportional to q, so let us try

$$U = q\left(\phi(\vec{r},t) + \vec{v}\cdot\vec{C}(\vec{r},t)\right).$$

Then we need to have

$$\vec{E} + \frac{\vec{v}}{c} \times \vec{B} = \frac{d}{dt}\vec{C} - \vec{\nabla}\phi - \sum_j v_j \vec{\nabla} C_j. \tag{2.19}$$

The first term is a stream derivative evaluated at the time-dependent position of the particle, so, as in Eq. (2.5),

$$\frac{d}{dt}\vec{C} = \frac{\partial \vec{C}}{\partial t} + \sum_j v_j \frac{\partial \vec{C}}{\partial x_j}.$$

The last term looks like the last term of (2.19), except that the indices on the derivative operator and on $\vec{C}$ have been reversed. This suggests that these two terms combine to form a cross product. Indeed, noting (B.10) that

$$\vec{v} \times \left(\vec{\nabla} \times \vec{C}\right) = \sum_j v_j \vec{\nabla} C_j - \sum v_j \frac{\partial \vec{C}}{\partial x_j},$$

[9] We have used Gaussian units here, but those who prefer S. I. units (rationalized MKS) can simply set $c = 1$.

we see that (2.19) becomes

$$\vec{E}+\frac{\vec{v}}{c}\times\vec{B}=\frac{\partial\vec{C}}{\partial t}-\vec{\nabla}\phi-\sum_j v_j\vec{\nabla}C_j+\sum_j v_j\frac{\partial\vec{C}}{\partial x_j}=\frac{\partial\vec{C}}{\partial t}-\vec{\nabla}\phi-\vec{v}\times\left(\vec{\nabla}\times\vec{C}\right).$$

We have successfully generated the term linear in $\vec{v}$ if we can show that there exists a vector field $\vec{C}(\vec{r},t)$ such that $\vec{B}=-c\vec{\nabla}\times\vec{C}$. A curl is always divergenceless, so this requires $\vec{\nabla}\cdot\vec{B}=0$, but this is indeed one of Maxwell's equations, and it ensures[10] there exists a vector field $\vec{A}$, known as the **magnetic vector potential**, such that $\vec{B}=\vec{\nabla}\times\vec{A}$. Thus with $\vec{C}=-\vec{A}/c$, we need only to find a ϕ such that

$$\vec{E}=-\vec{\nabla}\phi-\frac{1}{c}\frac{\partial\vec{A}}{\partial t}.$$

Once again, one of Maxwell's laws,

$$\vec{\nabla}\times\vec{E}+\frac{1}{c}\frac{\partial\vec{B}}{\partial t}=0,$$

gaurantees the existence of ϕ, the **electrostatic potential**, because after inserting $\vec{B}=\vec{\nabla}\times\vec{A}$, this is a statement that $\vec{E}+(1/c)\partial\vec{A}/\partial t$ has no curl, and is the gradient of something.

Thus we see that the Lagrangian which describes the motion of a charged particle in an electromagnetic field is given by a velocity-dependent potential

$$U(\vec{r},\vec{v})=q\left(\phi(r,t)-(\vec{v}/c)\cdot\vec{A}(\vec{r},t)\right).$$

Note, however, that this Lagrangian describes only the motion of the charged particle, and not the dynamics of the field itself.

Arbitrariness in the Lagrangian In this discussion of finding the Lagrangian to describe the Lorentz force, we used the lemma that guaranteed that the divergenceless magnetic field $\vec{B}$ can be written in terms

[10]This is but one of many consequences of the Poincaré lemma, discussed in section 6.5 (well, it should be). The particular forms we are using here state that if $\vec{\nabla}\cdot\vec{B}=0$ and $\vec{\nabla}\times\vec{F}=0$ in all of $\mathbb{R}^3$, then there exist a scalar function ϕ and a vector field $\vec{A}$ such that $\vec{B}=\vec{\nabla}\times\vec{A}$ and $\vec{F}=\vec{\nabla}\phi$.

of some magnetic vector potential $\vec{A}$, with $\vec{B} = \vec{\nabla} \times \vec{A}$. But $\vec{A}$ is not uniquely specified by $\vec{B}$; in fact, if a change is made, $\vec{A} \to \vec{A} + \vec{\nabla}\lambda(\vec{r}, t)$, $\vec{B}$ is unchanged because the curl of a gradient vanishes. The electric field $\vec{E}$ will be changed by $-(1/c)\partial\vec{A}/\partial t$, however, unless we also make a change in the electrostatic potential, $\phi \to \phi - (1/c)\partial\lambda/\partial t$. If we do, we have completely unchanged electromagnetic fields, which is where the physics lies. This change in the potentials,

$$\vec{A} \to \vec{A} + \vec{\nabla}\lambda(\vec{r}, t), \qquad \phi \to \phi - (1/c)\partial\lambda/\partial t, \tag{2.20}$$

is known as a **gauge transformation**, and the invariance of the physics under this change is known as **gauge invariance**. Under this change, the potential U and the Lagrangian are not unchanged,

$$L \to L - q\left(\delta\phi - \frac{\vec{v}}{c} \cdot \delta\vec{A}\right) = L + \frac{1}{c}\frac{\partial\lambda}{\partial t} - \vec{v} \cdot \vec{\nabla}\lambda(\vec{r}, t) = L + \frac{q}{c}\frac{d\lambda}{dt}.$$

We have here an example which points out that there is not a unique Lagrangian which describes a given physical problem, and the ambiguity is more that just the arbitrary constant we always knew was involved in the potential energy. This ambiguity is quite general, not depending on the gauge transformations of Maxwell fields. In general, if

$$L^{(2)}(q_j, \dot{q}_j, t) = L^{(1)}(q_j, \dot{q}_j, t) + \frac{d}{dt}f(q_j, t) \tag{2.21}$$

then $L^{(1)}$ and $L^{(2)}$ give the same equations of motion, and therefore the same physics, for $q_j(t)$. While this can be easily checked by evaluating the Lagrange equations, it is best understood in terms of the variation of the action. For any path $q_j(t)$ between q_{jI} at $t = t_I$ to q_{jF} at $t = t_F$, the two actions are related by

$$\begin{aligned} S^{(2)} &= \int_{t_I}^{t_F} \left(L^{(1)}(q_j, \dot{q}_j, t) + \frac{d}{dt}f(q_j, t)\right) dt \\ &= S^{(1)} + f(q_{jF}, t_F) - f(q_{jI}, t_I). \end{aligned}$$

The variation of path that one makes to find the stationary action does not change the endpoints q_{jF} and q_{jI}, so the difference $S^{(2)} - S^{(1)}$ is a

constant independent of the trajectory, and a stationary trajectory for $S^{(2)}$ is clearly stationary for $S^{(1)}$ as well.

The conjugate momenta are affected by the change in Lagrangian, however, because $L^{(2)} = L^{(1)} + \sum_j \dot{q}_j \partial f/\partial q_j + \partial f/\partial t$, so

$$p_j^{(2)} = \frac{\partial L^{(2)}}{\partial \dot{q}_j} = p_j^{(1)} + \frac{\partial f}{\partial q_j}.$$

This ambiguity is not usually mentioned in elementary mechanics, because if we restict our attention to Lagrangians consisting of canonical kinetic energy and potentials which are velocity-independent, a change (2.21) to a Lagrangian $L^{(1)}$ of this type will produce an $L^{(2)}$ which is not of this type, unless f is independent of position q and leaves the momenta unchanged.

Dissipation Another familiar force which is velocity dependent is friction. Even the "constant" sliding friction met with in elementary courses depends on the direction, if not the magnitude, of the velocity. Friction in a viscous medium is often taken to be a force proportional to the velocity, $\vec{F} = -\alpha\vec{v}$. We saw above that a potential linear in velocities produces a force perpendicular to $\vec{v}$, and a term higher order in velocities will contribute to the acceleration. This situation cannot handled by Lagrange's equations. An extension to the Lagrange formalism, involving Rayleigh's dissipation function, is discussed in Ref. [4].

Exercises

2.1 (Galelean relativity): Sally is sitting in a railroad car observing a system of particles, using a Cartesian coordinate system so that the particles are at positions $\vec{r}_i^{(S)}(t)$, and move under the influence of a potential $U^{(S)}(\{\vec{r}_i^{(S)}\})$. Thomas is in another railroad car, moving with constant velocity $\vec{u}$ with respect to Sally, and so he describes the position of each particle as $\vec{r}_i^{(T)}(t) = \vec{r}_i^{(S)}(t) - \vec{u}t$. Each takes the kinetic energy to be of the standard form in his system, *i.e.* $T^{(S)} = \frac{1}{2}\sum m_i \left(\dot{\vec{r}}_i^{(S)}\right)^2$ and $T^{(T)} = \frac{1}{2}\sum m_i \left(\dot{\vec{r}}_i^{(T)}\right)^2$.

(a) Show that if Thomas assumes the potential function $U^{(T)}(\vec{r}^{(T)})$ to be the same as Sally's at the same physical points,

$$U^{(T)}(\vec{r}^{(T)}) = U^{(S)}(\vec{r}^{(T)} + \vec{u}t), \tag{2.22}$$

then the equations of motion derived by Sally and Thomas describe the same physics. That is, if $r_i^{(S)}(t)$ is a solution of Sally's equations, $r_i^{(T)}(t) = r_i^{(S)}(t) - \vec{u}t$ is a solution of Thomas'.
(b) show that if $U^{(S)}(\{\vec{r}_i\})$ is a function only of the displacements of one particle from another, $\{\vec{r}_i - \vec{r}_j\}$, then $U^{(T)}$ is the same function of its arguments as $U^{(S)}$, $U^{(T)}(\{\vec{r}_i\}) = U^{(S)}(\{\vec{r}_i\})$. This is a different statement than Eq. 2.22, which states that they agree at the same physical configuration. Show it will not generally be true if $U^{(S)}$ is not restricted to depend only on the differences in positions.
(c) If it is true that $U^{(S)}(\vec{r}) = U^{(T)}(\vec{r})$, show that Sally and Thomas derive the same equations of motion, which we call "form invariance" of the equations.
(d) Show that nonetheless Sally and Thomas disagree on the energy of a particular physical motion, and relate the difference to the total momentum. Which of these quantities are conserved?

2.2 In order to show that the shortest path in two dimensional Euclidean space is a straight line without making the assumption that Δx does not change sign along the path, we can consider using a parameter λ and describing the path by two functions $x(\lambda)$ and $y(\lambda)$, say with $\lambda \in [0, 1]$. Then

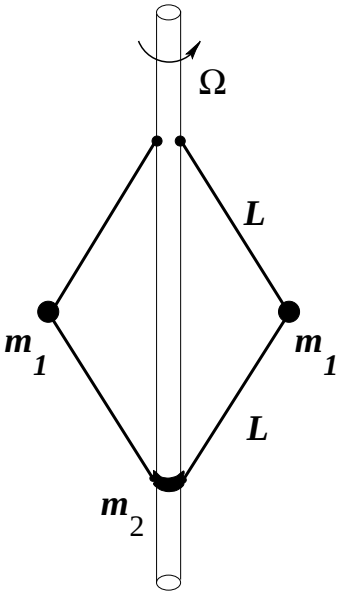
$$\ell = \int_0^1 d\lambda \sqrt{\dot{x}^2(\lambda) + \dot{y}^2(\lambda)},$$

where $\dot{x}$ means $dx/d\lambda$. This is of the form of a variational integral with two variables. Show that the variational equations do *not* determine the functions $x(\lambda)$ and $y(\lambda)$, but do determine that the path is a straight line. Show that the pair of functions $(x(\lambda), y(\lambda))$ gives the same action as another pair $(\tilde{x}(\lambda), \tilde{y}(\lambda))$, where $\tilde{x}(\lambda) = x(t(\lambda))$ and $\tilde{y}(\lambda) = y(t(\lambda))$, where $t(\lambda)$ is any monotone function mapping $[0, 1]$ onto itself. Explain why this equality of the lengths is obvious in terms of alternate parameterizations of the path. [In field theory, this is an example of a local gauge invariance, and plays a major role in string theory.]

2.3 Consider a circular hoop of radius R rotating about a vertical diameter at a fixed angular velocity Ω. On the hoop there is a bead of mass m, which

slides without friction on the hoop. The only external force is gravity. Derive the Lagrangian and the Lagrange equation using the polar angle θ as the unconstrained generalized coordinate. Find a conserved quantity, and find the equilibrium points, for which $\dot{\theta} = 0$. Find the condition on Ω such that there is an equilibrium point away from the axis.

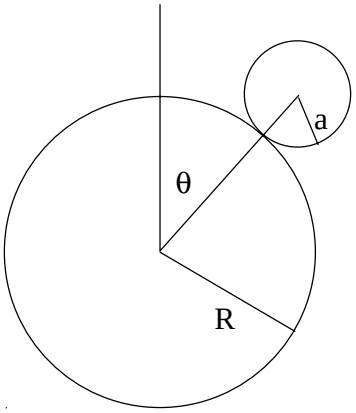
2.4 Early steam engines had a feedback device, called a governor, to automatically control the speed. The engine rotated a vertical shaft with an angular velocity Ω proportional to its speed. On opposite sides of this shaft, two hinged rods each held a metal weight, which was attached to another such rod hinged to a sliding collar, as shown.



Governor for a steam engine.

As the shaft rotates faster, the balls move outwards, the collar rises and uncovers a hole, releasing some steam. Assume all hinges are frictionless, the rods massless, and each ball has mass m_1 and the collar has mass m_2.
(a) Write the Lagrangian in terms of the generalized coordinate θ.
(b) Find the equilibrium angle θ as a function of the shaft angular velocity Ω. Tell whether the equilibrium is stable or not.

2.5 A cylinder of radius R is held horizontally in a fixed position, and a smaller uniform cylindrical disk of radius a is placed on top of the first cylinder, and is released from rest. There is a coefficient of static friction μ_s and a coefficient of kinetic friction $\mu_k < \mu_s$ for the contact between the cylinders. As the equilibrium at the top is unstable, the top cylinder will begin to roll on the bottom cylinder.



A small cylinder rolling on a fixed larger cylinder.

(a) If μ_s is sufficiently large, the small disk will roll until it separates from the fixed cylinder. Find the angle θ at which the separation occurs, and find the minimum value of μ_s for which this situation holds.
(b) If μ_s is less than the minimum value found above, what happens differently, and at what angle θ does this different behavior begin?

2.6 (a) Show that if $\Phi(q_1, ..., q_n, t)$ is an arbitrary differentiable function on extended configuration space, and $L^{(1)}(\{q_i\}, \{\dot{q}_j\}, t)$ and $L^{(2)}(\{q_i\}, \{\dot{q}_j\}, t)$ are two Lagrangians which differ by the total time derivative of Φ,

$$L^{(1)}(\{q_i\}, \{\dot{q}_j\}, t) = L^{(2)}(\{q_i\}, \{\dot{q}_j\}, t) + \frac{d}{dt}\Phi(q_1, ..., q_n, t),$$

show by explicit calculations that the equations of motion determined by $L^{(1)}$ are the same as the equations of motion determined by $L^{(2)}$.
(b) What is the relationship between the momenta $p_i^{(1)}$ and $p_i^{(2)}$ determined by these two Lagrangians respectively.

2.7 A particle of mass m lies on a frictionless horizontal table with a tiny hole in it. An inextensible massless string attached to m goes through the hole and is connected to another particle of mass M, which moves vertically only. Give a full set of generalized unconstrained coordinates and write the Lagrangian in terms of these. Assume the string remains taut at all times and that the motions in question never have either particle reaching the hole, and there is no friction of the string sliding at the hole.
Are there ignorable coordinates? Reduce the problem to a single second order differential equation.

2.8 Consider a mass m on the end of a massless rigid rod of length ℓ, the other end of which is free to rotate about a fixed point. This is a spherical pendulum. Find the Lagrangian and the equations of motion.

2.9 (a) Find a differential equation for $\theta(\phi)$ for the shortest path on the surface of a sphere between two arbitrary points on that surface, by minimizing the length of the path, assuming it to be monotone in ϕ.
(b) By geometrical argument (that it must be a great circle) argue that the path should satisfy

$$\cos(\phi - \phi_0) = K \cot\theta,$$

and show that this is indeed the solution of the differential equation you derived.

2.10 (a): Find the canonical momenta for a charged particle moving in an electromagnetic field and also under the influence of a non-electromagnetic force described by a potential $U(\vec{r})$.
(b): If the electromagnetic field is a constant magnetic field $\vec{B} = B_0\hat{e}_z$, with no electric field and with $U(\vec{r}) = 0$, what conserved quantities are there?

Chapter 3

Two Body Central Forces

Consider two particles of masses m_1 and m_2, with the only forces those of their mutual interaction, which we assume is given by a potential which is a function only of the distance between them, $U(|\vec{r}_1 - \vec{r}_2|)$. In a mathematical sense this is a very strong restriction, but it applies very nicely to many physical situations. The classical case is the motion of a planet around the Sun, ignoring the effects mentioned at the beginning of the book. But it also applies to electrostatic forces and to many effective representations of nonrelativistic interparticle forces.

3.1 Reduction to a one dimensional problem

Our original problem has six degrees of freedom, but because of the symmetries in the problem, many of these can be simply separated and solved for, reducing the problem to a mathematically equivalent problem of a single particle moving in one dimension. First we reduce it to a one-body problem, and then we reduce the dimensionality.

3.1.1 Reduction to a one-body problem

As there are no external forces, we expect the center of mass coordinate to be in uniform motion, and it behoves us to use

$$\vec{R} = \frac{m_1\vec{r}_1 + m_2\vec{r}_2}{m_1 + m_2}$$

as three of our generalized coordinates. For the other three, we first use the cartesian components of the relative coordinate

$$\vec{r} := \vec{r}_2 - \vec{r}_1,$$

although we will soon change to spherical coordinates for this vector. In terms of $\vec{R}$ and $\vec{r}$, the particle positions are

$$\vec{r}_1 = \vec{R} - \frac{m_2}{M}\vec{r}, \qquad \vec{r}_2 = \vec{R} + \frac{m_1}{M}\vec{r}, \qquad \text{where} \quad M = m_1 + m_2.$$

The kinetic energy is

$$\begin{aligned} T &= \frac{1}{2}m_1\dot{r}_1^2 + \frac{1}{2}m_2\dot{r}_2^2 \\ &= \frac{1}{2}m_1\left(\dot{\vec{R}} - \frac{m_2}{M}\dot{\vec{r}}\right)^2 + \frac{1}{2}m_2\left(\dot{\vec{R}} + \frac{m_1}{M}\dot{\vec{r}}\right)^2 \\ &= \frac{1}{2}(m_1 + m_2)\dot{\vec{R}}^2 + \frac{1}{2}\frac{m_1 m_2}{M}\dot{\vec{r}}^2 \\ &= \frac{1}{2}M\dot{\vec{R}}^2 + \frac{1}{2}\mu\dot{\vec{r}}^2, \end{aligned}$$

where

$$\mu := \frac{m_1 m_2}{m_1 + m_2}$$

is called the **reduced mass**. Thus the kinetic energy is transformed to the form for two effective particles of mass M and μ, which is neither simpler nor more complicated than it was in the original variables.

For the potential energy, however, the new variables are to be preferred, for $U(|\vec{r}_1 - \vec{r}_2| = U(|\vec{r}|)$ is independent of $\vec{R}$, whose three components are therefore ignorable coordinates, and their conjugate momenta

$$\left(\vec{P}_{cm}\right)_i = \frac{\partial(T-U)}{\partial\dot{R}_i} = M\dot{R}_i$$

are conserved. This reduces half of the motion to triviality, leaving an effective one-body problem with $T = \frac{1}{2}\mu\dot{r}^2$, and the given potential $U(\vec{r})$.

We have not yet made use of the fact that U only depends on the *magnitude* of $\vec{r}$. In fact, the above reduction applies to any two-body system without external forces, as long as Newton's Third Law holds.

3.1.2 Reduction to one dimension

In the problem under discussion, however, there is the additional restriction that the potential depends only on the magnitude of $\vec{r}$, that is, on the distance between the two particles, and not on the direction of $\vec{r}$. Thus we now convert from cartesian to spherical coordinates (r, θ, ϕ) for $\vec{r}$. In terms of the cartesian coordinates (x, y, z)

$$\begin{array}{ll} r = (x^2 + y^2 + z^2)^{\frac{1}{2}} & x = r\sin\theta\cos\phi \\ \theta = \cos^{-1}(z/r) & y = r\sin\theta\sin\phi \\ \phi = \tan^{-1}(y/x) & z = r\cos\theta \end{array}$$

Plugging into the kinetic energy is messy but eventually reduces to a rather simple form

$$\begin{aligned} T &= \frac{1}{2}\mu\left[\dot{x}_1^2 + \dot{x}_2^2 + \dot{x}_3^2\right] \\ &= \frac{1}{2}\mu\Big[(\dot{r}\sin\theta\cos\phi + \dot{\theta}r\cos\theta\cos\phi - \dot{\phi}r\sin\theta\sin\phi)^2 \\ &\quad +(\dot{r}\sin\theta\sin\phi + \dot{\theta}r\cos\theta\sin\phi + \dot{\phi}r\sin\theta\cos\phi)^2 \\ &\quad +(\dot{r}\cos\theta - \dot{\theta}r\sin\theta)^2\Big] \\ &= \frac{1}{2}\mu\left[\dot{r}^2 + r^2\dot{\theta}^2 + r^2\sin^2\theta\dot{\phi}^2\right] \end{aligned} \tag{3.1}$$

Notice that in spherical coordinates T is a funtion of r and θ as well as $\dot{r}$, $\dot{\theta}$, and $\dot{\phi}$, but it is not a function of ϕ, which is therefore an ignorable coordinate, and

$$P_\phi = \frac{\partial L}{\partial\dot{\phi}} = \mu r^2\sin^2\theta\dot{\phi} = \text{ constant.}$$

Note that $r\sin\theta$ is the distance of the particle from the z-axis, so P_ϕ is just the z-component of the angular momentum, L_z. Of course all

of $\vec{L} = \vec{r} \times \vec{p}$ is conserved, because in our effective one body problem there is no torque about the origin. Thus $\vec{L}$ is a constant[1], and the motion must remain in a plane perpendicular to $\vec{L}$ and passing through the origin, as a consequence of the fact that $\vec{r} \perp \vec{L}$. It simplifies things if we choose our coordinates so that $\vec{L}$ is in the z-direction. Then $\theta = \pi/2, \dot{\theta} = 0, L = \mu r^2 \dot{\phi}$. The r equation of motion is then

$$\mu \ddot{r} - \mu r \dot{\phi}^2 + dU/dr = 0 = \mu \ddot{r} - \frac{L^2}{\mu r^3} + dU/dr.$$

This is the one-dimensional motion of body in an effective potential

$$U_{\text{eff}}(r) = U(r) + \frac{L^2}{2\mu r^2}.$$

Thus we have reduced a two-body three-dimensional problem to one with a single degree of freedom, without any additional complication except the addition of a **centrifugal barrier** term $L^2/2\mu r^2$ to the potential.

Before we proceed, a comment may be useful in retrospect about the reduction in variables in going from the three dimensional one-body problem to a one dimensional problem. Here we reduced the phase space from six variables to two, in a problem which had four conserved quantities, $\vec{L}$ and H. But we have not yet used the conservation of H in this reduction, we have only used the three conserved quantities $\vec{L}$. Where have these dimensions gone? From $\vec{L}$ conservation, by choosing our axes with $\vec{L} \parallel z$, the two constraints $L_x = 0$ and $L_y = 0$ (with $L_z \neq 0$) do imply $z = p_z = 0$, thereby eliminating two of the coordinates of phase space. The conservation of L_z, however, is a consequence of an ignorable coordinate ϕ, with conserved conjugate momentum $P_\phi = L_z$. In this case, not only is the corresponding momentum restricted to a constant value, eliminating one dimension of variation in phase space, but the corresponding coordinate, ϕ, while not fixed, drops out of consideration because it does not appear in the remaining one dimensional

[1]If $\vec{L} = 0$, $\vec{p}$ and $\vec{r}$ are in the same direction, to which the motion is then confined. In this case it is more appropriate to use Cartesian coordinates with this direction as x, reducing the problem to a one-dimensional problem with potential $U(x) = U(r = |x|)$. In the rest of this chapter we assume $\vec{L} \neq 0$.

problem. This is generally true for an ignorable coordinate — the corresponding momentum becomes a time-constant parameter, and the coordinate disappears from the remaining problem.

3.2 Integrating the motion

We can simplify the problem even more by using the one conservation law left, that of energy. Because the energy of the effective motion is a constant,

$$E = \frac{1}{2}\mu\dot{r}^2 + U_{\text{eff}} = \text{ constant}$$

we can immediately solve for

$$\frac{dr}{dt} = \pm\left\{\frac{2}{\mu}\left(E - U_{\text{eff}}(r)\right)\right\}^{1/2}.$$

This can be inverted and integrated over r, to give

$$t = t_0 \pm \int \frac{dr}{\sqrt{2\left(E - U_{\text{eff}}(r)\right)/\mu}}, \tag{3.2}$$

which is the inverse function of the solution to the radial motion problem $r(t)$. We can also find the orbit because

$$\frac{d\phi}{dr} = \frac{\dot{\phi}}{dr/dt} = \frac{L}{\mu r^2}\frac{dt}{dr}$$

so

$$\phi = \phi_0 \pm L\int_{r_0}^{r} \frac{dr}{r^2\sqrt{2\mu\left(E - U_{\text{eff}}(r)\right)}}. \tag{3.3}$$

The sign ambiguity from the square root is only because r may be increasing or decreasing, but time, and usually ϕ/L, are always increasing.

Qualitative features of the motion are largely determined by the range over which the argument of the square root is positive, as for

other values of r we would have imaginary velocities. Thus the motion is restricted to this allowed region. Unless $L = 0$ or the potential $U(r)$ is very strongly attractive for small r, the centrifugal barrier will dominate, so $U_{\text{eff}} \underset{r\to 0}{\longrightarrow} +\infty$, and there must be a smallest radius $r_p > 0$ for which $E \geq U_{\text{eff}}$. Generically the force will not vanish there, so $E - U_{\text{eff}} \approx c(r - r_p)$ for $r \approx r_p$, and the integrals in (3.2) and (3.3) are convergent. Thus an incoming orbit reaches $r = r_p$ at a finite time and finite angle, and the motion then continues with r increasing and the $\pm$ signs reversed. The radius r_p is called a **turning point** of the motion. If there is also a maximum value of r for which the velocity is real, it is also a turning point, and an outgoing orbit will reach this maximum and then r will start to decrease, confining the orbit to the allowed values of r.

If there are both minimum and maximum values, this interpretation of Eq. (3.3) gives ϕ as a multiple valued function of r, with an "inverse" $r(\phi)$ which is a periodic function of ϕ. But there is no particular reason for this period to be the geometrically natural periodicity 2π of ϕ, so that different values of r may be expected in successive passes through the same angle in the plane of the motion. There would need to be something very special about the attractive potential for the period to turn out to be just 2π, but indeed that is the case for Newtonian gravity.

We have reduced the problem of the motion to doing integrals. In general that is all we can do explicitly, but in some cases we can do the integral analytically, and two of these special cases are very important physically.

3.2.1 The Kepler problem

Consider first the force of Newtonian gravity, or equivalently the Coulomb attraction of unlike charged particles. The force $F(r) = -K/r^2$ has a potential

$$U(r) = -\frac{K}{r}.$$

Then the ϕ integral is

$$\begin{aligned} \phi &= \phi_0 \pm \int \frac{L}{\mu r^2} dr \left\{ \frac{2E}{\mu} + \frac{2K}{r} - \frac{L^2}{\mu^2 r^2} \right\}^{-1/2} \\ &= \phi_0 \pm \int \frac{du}{\sqrt{\gamma + \alpha u - u^2}} \end{aligned} \tag{3.4}$$

where we have made the variable substitution $u = 1/r$ which simplifies the form, and have introduced abbreviations $\gamma = 2\mu E/L^2$, $\alpha = 2K\mu/L^2$.

As $d\phi/dr$ must be real the motion will clearly be confined to regions for which the argument of the square root is nonnegative, and the motion in r will reverse at the turning points where the argument vanishes. The argument is clearly negative as $u \to \infty$, which is $r = 0$. We have assumed $L \neq 0$, so the angular momentum barrier dominates over the Coulomb attraction, and always prevents the particle from reaching the origin. Thus there is always at least one turning point, $u_{\max}$, corresponding to the minimum distance $r_{\min}$. Then the argument of the square root must factor into $[-(u - u_{\max})(u - u_{\min})]$, although if $u_{\min}$ is negative it is not really the minimum u, which can never get past zero. The integral (3.4) can be done[2] with the substitution $\sin^2 \beta = (u_{\max} - u)/(u_{\max} - u_{\min})$. This shows $\phi = \phi_0 \pm 2\beta$, where ϕ_0 is the angle at $r = r_{\min}$, $u = u_{\max}$. Then

$$u \equiv \frac{1}{r} = A \cos(\phi - \phi_0) + B$$

where A and B are constants which could be followed from our sequence of substitutions, but are better evaluated in terms of the conserved quantities E and L directly. $\phi = \phi_0$ corresponds to the minimum r, $r = r_p$, the point of closest approach, or perigee[3], so $r_p^{-1} = A + B$, and $A > 0$. Let $\theta = \phi - \phi_0$ be the angle from this minimum, with the x

[2]Of course it can also be done by looking in a good table of integrals. For example, see 2.261(c) of Gradshtein and Ryzhik[5].

[3]Perigee is the correct word if the heavier of the two is the Earth, perihelion if it is the sun, periastron for some other star. Pericenter is also used, but not as generally as it ought to be.

axis along $\theta = 0$. Then

$$\frac{1}{r} = A\cos\theta + B = \frac{1}{r_p}\left(1 - \frac{e}{1+e}(1-\cos\theta)\right) = \frac{1}{r_p}\frac{1+e\cos\theta}{1+e}$$

where $e = A/B$.

What is this orbit? Clearly r_p just sets the scale of the whole orbit. From $r_p(1+e) = r + er\cos\theta = r + ex$, if we subtract ex and square, we get $r_p^2 + 2r_p e(r_p - x) + e^2(r_p - x)^2 = r^2 = x^2 + y^2$, which is clearly quadratic in x and y. It is therefore a conic section,

$$y^2 + (1-e^2)x^2 + 2e(1+e)xr_p - (1+e)^2 r_p^2 = 0.$$

The nature of the curve depends on the coefficient of x^2. For

- $|e| < 1$, the coefficient is > 0, and we have an ellipse.
- $e = \pm 1$, the coefficient vanishes and $y^2 = ax + b$ is a parabola.
- $|e| > 1$, the coefficient is < 0, and we have a hyperbola.

All of these are posible motions. The bound orbits are ellipses, which describe planetary motion and also the motion of comets. But objects which have enough energy to escape from the sun, such as Voyager 2, are in hyperbolic orbit, or in the dividing case where the total energy is exactly zero, a parabolic orbit. Then as time goes to ∞, ϕ goes to a finite value, $\phi \to \pi$ for a parabola, or some constant less than π for a hyperbolic orbit.

Let us return to the elliptic case. The closest approach, or **perigee**, is $r = r_p$, while the furthest apart the objects get is at $\theta = \pi, r = r_a = r_p(1+e)/(1-e)$, which is called the **apogee** or aphelion. e is the **eccentricity** of the ellipse. An ellipse is a circle stretched uniformly in one direction; the diameter in that direction becomes the **major axis** of the ellipse, while the perpendicular diameter becomes the **minor axis**.

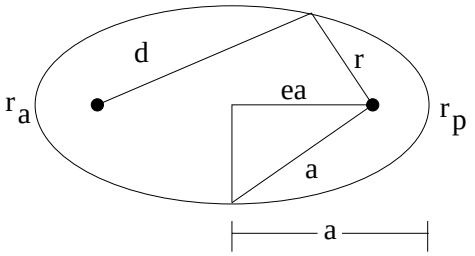
One half the length of the major axis is the **semi-major axis** and is denoted by a.

$$a = \frac{1}{2}\left(r_p + r_p\frac{1+e}{1-e}\right) = \frac{r_p}{1-e},$$

so

$$r_p = (1-e)a, \qquad r_a = (1+e)a.$$

Notice that the center of the ellipse is ea away from the Sun.



Properties of an ellipse. The large dots are the foci. The eccentricity is e and a is the semi-major axis

Kepler tells us not only that the orbit is an ellipse, but also that the sun is at one focus. To verify that, note the other focus of an ellipse is symmetrically located, at $(-2ea, 0)$, and work out the sum of the distances of any point on the ellipse from the two foci. This will verify that $d+r = 2a$ is a constant, showing that the orbit is indeed an ellipse with the sun at one focus.

How are a and e related to the total energy E and the angular momentum L? At apogee and perigee, $dr/d\phi$ vanishes, and so does $\dot{r}$, so $E = U(r) + L^2/2\mu r^2 = -K/r + L^2/2\mu r^2$, which holds at $r = r_p = a(1-e)$ and at $r = r_a = a(1+e)$. Thus $Ea^2(1\pm e)^2 + Ka(1\pm e) - L^2/2\mu = 0$. These two equations are easily solved for a and e in terms of the constants of the motion E and L

$$a = -\frac{K}{2E}, \qquad e^2 = 1 + \frac{2EL^2}{\mu K^2}.$$

As expected for a bound orbit, we have found r as a periodic function of ϕ, but it is surprising that the period is the natural period 2π. In other words, as the planet makes its revolutions around the sun, its perihelion is always in the same direction. That didn't have to be the case — one could imagine that each time around, the minimum distance occurred at a slightly different (or very different) angle. Such an effect is called the **precession of the perihelion**. We will discuss this for nearly circular orbits in other potentials in section (3.2.2).

What about Kepler's Third Law? The area of a triange with $\vec{r}$ as one edge and the displacement during a small time interval $\delta\vec{r} = \vec{v}\delta t$ is

$A = \frac{1}{2}|\vec{r} \times \vec{v}|\delta t = |\vec{r} \times \vec{p}|\delta t/2\mu$, so the area swept out per unit time is

$$\frac{dA}{dt} = \frac{L}{2\mu}.$$

which is constant. The area of an ellipse made by stretching a circle is stretched by the same amount, so A is π times the semimajor axis times the semiminor axis. The endpoint of the semiminor axis is a away from each focus, so it is $a\sqrt{1-e^2}$ from the center, and

$$\begin{aligned} A &= \pi a^2\sqrt{1-e^2} = \pi a^2\sqrt{1-\left(1+\frac{2EL^2}{\mu K^2}\right)} \\ &= \pi a^2 \frac{L}{K}\sqrt{\frac{-2E}{\mu}}. \end{aligned}$$

Recall that for bound orbits $E < 0$, so A is real. The period is just the area swept out in one revolution divided by the rate it is swept out, or

$$\begin{aligned} T &= \pi a^2 \frac{L}{K}\sqrt{\frac{-2E}{\mu}}\frac{2\mu}{L} \\ &= \frac{2\pi a^2}{K}\sqrt{-2\mu E} = \frac{\pi}{2}K(2\mu)^{1/2}(-E)^{-3/2} \qquad (3.5) \\ &= \frac{2\pi a^2}{K}\sqrt{\mu K/a} = 2\pi a^{3/2}(K)^{-1/2}\mu^{1/2}, \qquad (3.6) \end{aligned}$$

independent of L. The fact that T and a depend only on E and not on L is another fascinating manifestation of the very subtle symmetries of the Kepler/Coulomb problem.

3.2.2 Nearly Circular Orbits

For a general central potential we cannot find an analytic form for the motion, which involves solving the effective one-dimensional problem with $U_{\text{eff}}(r) = U(r) + L^2/2\mu r^2$. If $U_{\text{eff}}(r)$ has a minimum at $r = a$, one solution is certainly a circular orbit of radius a. The minimum requires $dU_{\text{eff}}(r)/dr = 0 = -F(r) - L^2/\mu r^3$, so

$$F(a) = -\frac{L^2}{\mu a^3}.$$

We may also ask about trajectories which differ only slightly from this orbit, for which $|r-a|$ is small. Expanding $U_{\rm eff}(r)$ in a Taylor series about a,

$$U_{\rm eff}(r) = U_{\rm eff}(a) + \frac{1}{2}(r-a)^2 k,$$

where

$$\begin{aligned} k &= \left.\frac{d^2 U_{\rm eff}}{dr^2}\right|_a \\ &= -\frac{dF}{dr} + \frac{3L^2}{\mu a^4} = -\left(\frac{dF}{dr} + \frac{3F}{a}\right). \end{aligned}$$

For $r=a$ to be a minimum and the nearly circular orbits to be stable, the second derivative and k must be positive, and therefore $F'+3F/a < 0$. As always when we treat a problem as small deviations from a stable equilibrium[4] we have harmonic oscillator motion, with a period $T_{\rm osc} = 2\pi\sqrt{\mu/k}$.

As a simple class of examples, consider the case where the force law depends on r with a simple power, $F=-cr^n$. Then $k=(n+3)ca^{n-1}$, which is positive and the orbit stable only if $n > -3$. For gravity, $n=-2, c=K, k=K/a^3$, and

$$T_{\rm osc} = 2\pi\sqrt{\frac{\mu a^3}{K}}$$

agreeing with what we derived for the more general motion, not restricted to small deviations from circularity. But for more general n, we find

$$T_{\rm osc} = 2\pi\sqrt{\frac{\mu a^{1-n}}{c(n+3)}}.$$

The period of revolution $T_{\rm rev}$ can be calculated for the circular orbit, as

$$L = \mu a^2\dot\theta = \mu a^2 \frac{2\pi}{T_{\rm rev}} = \sqrt{\mu a^3 |F(a)|},$$

[4]This statement has an exception if the second derivative vanishes, $k=0$.

so

$$T_{\rm rev} = 2\pi\sqrt{\frac{\mu a}{|F(a)|}}$$

which for the power law case is

$$T_{\rm rev} = 2\pi\sqrt{\frac{\mu a^{1-n}}{c}}.$$

Thus the two periods $T_{\rm osc}$ and $T_{\rm rev}$ are not equal unless $n = -2$, as in the gravitational case. Let us define the **apsidal angle** ψ as the angle between an apogee and the next perigee. It is therefore $\psi = \pi T_{\rm osc}/T_{\rm rev} = \pi/\sqrt{3+n}$. For the gravitational case $\psi = \pi$, the apogee and perigee are on opposite sides of the orbit. For a two- or three-dimensional harmonic oscillator $F(r) = -kr$ we have $n = 1, \psi = \frac{1}{2}\pi$, and now an orbit contains two apogees and two perigees, and is again an ellipse, but now with the center-of-force at the center of the ellipse rather than at one focus.

Note that if ψ/π is not rational, the orbit never closes, while if $\psi/\pi = p/q$, the orbit will close after q revolutions, having reached p apogees and perigees. The orbit will then be closed, but unless $q = 1$ it will be self-intersecting. This exact closure is also only true in the small deviation approximation; more generally, Bertrand's Theorem states that only for the $n = -2$ and $n = 1$ cases are the generic orbits closed.

In the treatment of planetary motion, the precession of the perihelion is the angle though which the perihelion slowly moves, so it is $2\psi - 2\pi$ per orbit. We have seen that it is zero for the pure inverse force law. There is actually some precession of the planets, due mostly to perturbative effects of the other planets, but also in part due to corrections to Newtonian mechanics found from Einstein's theory of general relativity. In the late nineteenth century descrepancies in the precession of Mercury's orbit remained unexplained, and the resolution by Einstein was one of the important initial successes of general relativity.

3.3 The Laplace-Runge-Lenz Vector

The remarkable simplicity of the motion for the Kepler and harmonic oscillator central force problems is in each case connected with a hidden symmetry. We now explore this for the Kepler problem.

For any central force problem $\vec{F} = \dot{\vec{p}} = f(r)\hat{e}_r$ we have a conserved angular momentum $\vec{L} = m(\vec{r} \times \dot{\vec{r}})$, for $\dot{\vec{L}} = m\dot{\vec{r}} \times \dot{\vec{r}} + (f(r)/r)\vec{r} \times \vec{r} = 0$. The motion is therefore confined to a plane perpendicular to $\vec{L}$, and the vector $\vec{p} \times \vec{L}$ is always in the plane of motion, as are $\vec{r}$ and $\vec{p}$. Consider the evolution of $\vec{p} \times \vec{L}$ with time[5]

$$\begin{aligned} \frac{d}{dt}\left(\vec{p} \times \vec{L}\right) &= \dot{\vec{p}} \times \vec{L} = \vec{F} \times \vec{L} = mf(r)\hat{e}_r \times (\vec{r} \times \dot{\vec{r}}) \\ &= mf(r)\left(\vec{r}\hat{e}_r \cdot \dot{\vec{r}} - \dot{\vec{r}}\hat{e}_r \cdot \vec{r}\right) = mf(r)(\dot{r}\vec{r} - r\dot{\vec{r}}) \end{aligned}$$

On the other hand, the time variation of the unit vector $\hat{e}_r = \vec{r}/r$ is

$$\frac{d}{dt}\hat{e}_r = \frac{d}{dt}\frac{\vec{r}}{r} = \frac{\dot{\vec{r}}}{r} - \frac{\dot{r}\vec{r}}{r^2} = -\frac{\dot{r}\vec{r} - r\dot{\vec{r}}}{r^2}.$$

For the Kepler case, where $f(r) = -K/r^2$, these are proportional to each other with a constant ratio, so we can combine them to form a *conserved* quantity $\vec{A} = \vec{p} \times \vec{L} - mK\hat{e}_r$, called[6] the **Laplace-Runge-Lenz vector**, $d\vec{A}/dt = 0$.

While we have just found three conserved quantities in addition to the conserved energy and the three conserved components of $\vec{L}$, these cannot all be independent. Indeed we have already noted that $\vec{A}$ lies in the plane of motion and is perpendicular to $\vec{L}$, so $\vec{A} \cdot \vec{L} = 0$. If we dot $\vec{A}$ into the position vector,

$$\vec{A} \cdot \vec{r} = \vec{r} \cdot (\vec{p} \times (\vec{r} \times \vec{p})) - mkr = (\vec{r} \times \vec{p})^2 - mkr = L^2 - mkr,$$

so if θ is the angle between $\vec{A}$ and $\vec{r}$, we have $Ar\cos\theta + mkr = L^2$, or

$$\frac{1}{r} = \frac{mk}{L^2}\left(1 + \frac{A}{mk}\cos\theta\right),$$

[5]Some hints: $\vec{A} \times (\vec{B} \times \vec{C}) = \vec{B}(\vec{A} \cdot \vec{C}) - \vec{C}(\vec{A} \cdot \vec{B})$, and $\hat{e}_r \cdot \dot{\vec{r}} = (1/r)\vec{r} \cdot \dot{\vec{r}} = (1/2r)d(r^2)/dt = \dot{r}$. The first equation, known as the **bac-cab** equation, is shown in Appendix A.

[6]by Goldstein, at least. While others often use only the last two names, Laplace clearly has priority.

which is an elegant way of deriving the formula we found previously by integration, with $A = mke$. Note $\theta = 0$ is the perigee, so $\vec{A}$ is a constant vector pointing towards the perigee.

We also see that the magnitude of $\vec{A}$ is given in terms of e, which we have previously related to L and E, so $A^2 = m^2k^2 + 2mEL^2$ is a further relation among the seven conserved quantities, showing that only five are independent. There could not be more than five independent conserved functions depending analytically on the six variables of phase space (for the relative motion only), for otherwise the point representing the system in phase space would be unable to move. In fact, the five independent conserved quantities on the six dimensional dimensional phase space confine a generic invariant set of states, or orbit, to a one dimensional subspace. For power laws other than $n = -2$ and $n = 1$, as the orbits do not close, they are dense in a two dimensional region of phase space, indicating that there cannot be more than four independent conserved analytic functions on phase space. So we see the connection between the existence of the conserved $\vec{A}$ in the Kepler case and the fact that the orbits are closed.

3.4 The virial theorem

Consider a system of particles and the quantity $G = \sum_i \vec{p}_i \cdot \vec{r}_i$. Then the rate at which this changes is

$$\frac{dG}{dt} = \sum \vec{F}_i \cdot \vec{r}_i + 2T.$$

If the system returns to a region in phase space where it had been, after some time, G returns to what it was, and the average value of dG/dt vanishes,

$$\left\langle \frac{dG}{dt} \right\rangle = \left\langle \sum \vec{F}_i \cdot \vec{r}_i \right\rangle + 2 \langle T \rangle = 0.$$

This average will also be zero if the region stays in some bounded part of phase space for which G can only take bounded values, and the averaging time is taken to infinity. This is appropriate for a system in thermal equilibrium, for example.

Consider a gas of particles which interact only with the fixed walls of the container, so that the force acts only on the surface, and the sum becomes an integral over $d\vec{F} = -pd\vec{A}$, where p is the uniform pressure and $d\vec{A}$ is an outward pointing vector representing a small piece of the surface of the volume. Then

$$\left\langle \sum \vec{F}_i \cdot \vec{r}_i \right\rangle = -\int_{\delta V} p\vec{r} \cdot d\vec{A} = -p \int_V \nabla \cdot \vec{r} dV = -3pV$$

so $\langle 2T \rangle = 3pV$.

A very different application occurs for a power law central force between pairs of particles, say for a potential $U(\vec{r}_i, \vec{r}_j) = a|\vec{r}_i - \vec{r}_j|^{n+1}$. Then this action and reaction contribute $\vec{F}_{ij} \cdot \vec{r}_j + \vec{F}_{ji} \cdot \vec{r}_i = \vec{F}_{ji} \cdot (\vec{r}_i - \vec{r}_j) = -(n+1)a|\vec{r}_i - \vec{r}_j|^{n+1} = -(n+1)U(\vec{r}_i, \vec{r}_j)$. So summing over all the particles and using $\langle 2T \rangle = -\langle \sum \vec{F} \cdot \vec{r} \rangle$, we have

$$\langle T \rangle = \frac{n+1}{2} \langle U \rangle.$$

For Kepler, $n = -2$, so $\langle T \rangle = -\frac{1}{2}\langle U \rangle = -\langle T + U \rangle = -E$ must hold for closed orbits or for large systems of particles which remain bound and uncollapsed. It is not true, of course, for unbound systems which have $E > 0$.

The fact that the average value of the kinetic energy in a bound system gives a measure of the potential energy is the basis of the measurements of the missing mass, or dark matter, in galaxies and in clusters of galaxies. This remains a useful tool despite the fact that a multiparticle gravitationally bound system can generally throw off some particles by bringing others closer together, so that, strictly speaking, G does not return to its original value or remain bounded.

3.5 Rutherford Scattering

We have discussed the $1/r$ potential in terms of Newtonian gravity, but of course it is equally applicable to Coulomb's law of electrostatic

forces. The force between nonrelativistic charges Q and q is given[7] by

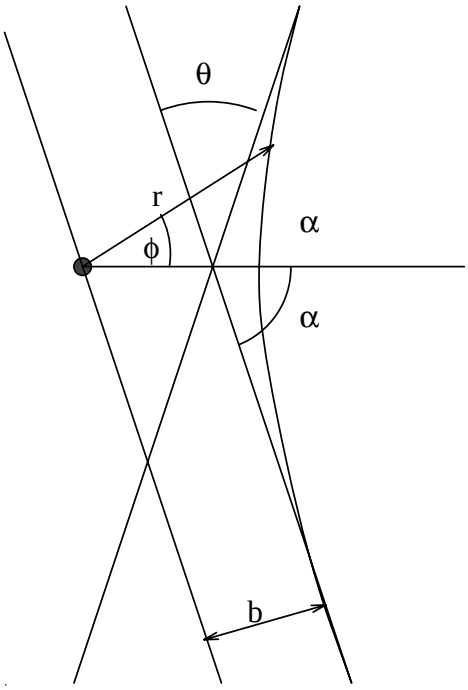
$$\vec{F} = \frac{1}{4\pi\epsilon_0}\frac{Qq}{r^3}\vec{r},$$

and the potential energy is $U(r) = -K/r$ with $K = -Qq/4\pi\epsilon_0$.

Unlike gravity, the force is not always attractive ($K > 0$), and for like sign charges we have $K < 0$, and therefore U and the total energy are always positive, and there are no bound motions. Whatever the relative signs, we are going to consider scattering here, and therefore positive energy solutions with the initial state of finite speed v_0 and $r \to \infty$. Thus the relative motion is a hyperbola, with

$$\begin{aligned} r &= r_p\frac{1+e}{1+e\cos\phi} \\ e &= \pm\sqrt{1+\frac{2EL^2}{\mu K^2}}. \end{aligned}$$

This starts and ends with $r \to \infty$, at $\phi \to \pm\alpha = \pm\cos^{-1}(-1/e)$, and the angle θ through which the velocity changes is called the **scattering angle**. For simplicity we will consider the repulsive case, with $e < 0$ so that $\alpha < \pi/2$.



Rutherford scattering. An α particle approaches a heavy nucleus with an impact parameter b, scattering through an angle θ. The cross sectional area $d\sigma$ of the incident beam is scattered through angles $\in [\theta, \theta + d\theta]$.

[7] Here we use S. I. or rationalized MKS units. For Gaussian units drop the $4\pi\epsilon_0$, or for Heaviside-Lorentz units drop only the ϵ_0.

We see that $\theta = \pi - 2\alpha$, so

$$\tan\frac{\theta}{2} = \cot\alpha = \frac{\cos\alpha}{\sqrt{1-\cos^2\alpha}} = \frac{|e|^{-1}}{\sqrt{1-|e|^{-2}}} = \frac{1}{\sqrt{e^2-1}} = \sqrt{\frac{\mu K^2}{2EL^2}}.$$

We have $K = Qq/4\pi\epsilon_0$. We need to evaluate E and L. At $r = \infty$, $U \to 0$, $E = \frac{1}{2}\mu v_0^2$, $L = \mu b v_0$, where b is the **impact parameter**, the distance by which the asymptotic line of the initial motion misses the scattering center. Thus

$$\tan\frac{\theta}{2} = K\sqrt{\frac{\mu}{\mu v_0^2(\mu b v_0)^2}} = \frac{K}{\mu b v_0^2}. \tag{3.7}$$

The scattering angle therefore depends on b, the perpendicular displacement from the axis parallel to the beam through the nucleus. Particles passing through a given area will be scattered through a given angle, with a fixed angle θ corresponding to a circle centered on the axis, having radius $b(\theta)$ given by 3.7. The area of the beam $d\sigma$ in an annular ring of impact parameters $\in [b, b+db]$ is $d\sigma = 2\pi b db$. To relate db to $d\theta$, we differentiate the scattering equation for fixed v_0,

$$\frac{1}{2}\sec^2\frac{\theta}{2}d\theta = \frac{-K}{\mu v_0^2 b^2}db,$$

$$\begin{aligned}
\frac{d\sigma}{d\theta} &= 2\pi b\frac{\mu v_0^2 b^2}{2K\cos^2(\theta/2)} = \frac{\pi\mu v_0^2 b^3}{K\cos^2(\theta/2)} \\
&= \frac{\pi\mu v_0^2}{K\cos^2(\theta/2)}\left(\frac{K}{\mu v_0^2}\right)^3\left(\frac{\cos\theta/2}{\sin\theta/2}\right)^3 = \pi\left(\frac{K}{\mu v_0^2}\right)^2\frac{\cos\theta/2}{\sin^3\theta/2} \\
&= \frac{\pi}{2}\left(\frac{K}{\mu v_0^2}\right)^2\frac{\sin\theta}{\sin^4\theta/2}.
\end{aligned}$$

(The last expression is useful because $\sin\theta d\theta$ is the "natural measure" for θ, in the sense that integrating over volume in spherical coordinates is $d^3V = r^2 dr\sin\theta d\theta d\phi$.)

How do we measure $d\sigma/d\theta$? There is a beam of N particles shot at random impact parameters onto a foil with n scattering centers per

unit area, and we confine the beam to an area A. Each particle will be significantly scattered only by the scattering center to which it comes closest, if the foil is thin enough. The number of incident particles per unit area is N/A, and the number of scatterers being bombarded is nA, so the number which get scattered through an angle $\in [\theta, \theta + d\theta]$ is

$$\frac{N}{A} \times nA \times \frac{d\sigma}{d\theta} d\theta = Nn \frac{d\sigma}{d\theta} d\theta.$$

We have used the cylindrical symmetry of this problem to ignore the ϕ dependance of the scattering. More generally, the scattering would not be uniform in ϕ, so that the area of beam scattered into a given region of (θ,ϕ) would be

$$d\sigma = \frac{d\sigma}{d\Omega} \sin\theta d\theta d\phi,$$

where $d\sigma/d\Omega$ is called the **differential cross section**. For Rutherford scattering we have

$$\frac{d\sigma}{d\Omega} = \frac{1}{4} \left(\frac{K}{\mu v_0^2} \right)^2 \csc^4 \frac{\theta}{2}.$$

Scattering in other potentials

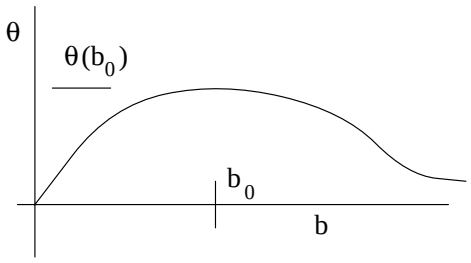
We see that the cross section depends on the angle through which the incident particle is scattered for a given impact parameter. In Rutherford scattering θ increases monotonically as b decreases, which is possible only because the force is "hard", and a particle aimed right at the center will turn around rather than plowing through. This was a surprize to Rutherford, for the concurrent model of the nucleus, Thompson's plum pudding model, had the nuclear charge spread out over some atomic-sized spherical region, and the Coulomb potential would have decreased once the alpha particle entered this region. So sufficiently energetic alpha particles aimed at the center should have passed through undeflected instead of scattered backwards. In fact, of course, the nucleus does have a finite size, and this is still true, but at a much smaller distance, and therefore a much larger energy.

If the scattering angle $\theta(b)$ does run smoothly from 0 at $b = 0$ to 0 at $b \to \infty$, as shown, then there is an extremal value for which

$d\theta/db|_{b_0} = 0$, and for $\theta < \theta(b_0)$, $d\sigma/d\theta$ can get contributions from several different b's,

$$\frac{d\sigma}{d\Omega} = \sum_i \frac{b_i}{\sin\theta} \left.\frac{db}{d\theta}\right|_i .$$

It also means that the cross section becomes infinite as $\theta \to \theta(b_0)$, and vanishes above that value of θ. This effect is known as **rainbow scattering**, and is the cause of rainbows, because the scattering for a given color light off a water droplet is very strongly peaked at the maximum angle of scattering.

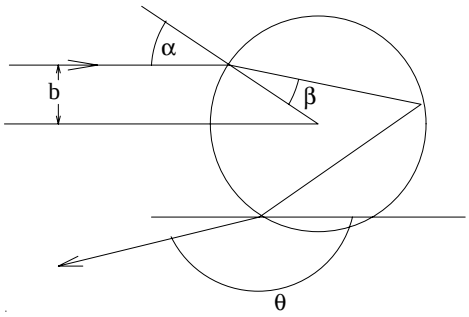


Another unusual effect occurs when $\theta(b)$ becomes 0 or π for some nonzero value of b, with $db/d\theta$ finite. Then $d\sigma/d\Omega$ blows up due to the $\sin\theta$ in the denominator, even though the integral $\int (d\sigma/d\Omega)\sin\theta d\theta d\phi$ is perfectly finite. This effect is called **glory scattering**, and can be seen around the shadow of a plane on the clouds below.

Exercises

3.1 Consider a spherical droplet of water in the sunlight. A ray of light with impact parameter b is refracted, so by Snell's Law $n\sin\beta = \sin\alpha$. It is then internally reflected once and refracted again on the way out.
(a) Express the scattering angle θ in terms of α and β.

(b) Find the scattering cross section $d\sigma/d\Omega$ as a function of θ, α and β (which is implicitly a function of θ from (a) and Snell's Law).
(c) The smallest value of θ is called the rainbow scattering angle. Why? Find it numerically to first order in δ if the index of refraction is $n = 1.333 + \delta$
(d) The visual spectrum runs from violet, where $n = 1.343$, to red, where $n = 1.331$. Find the angular radius of the rainbow's circle, and the angular width of the rainbow, and tell whether the red or blue is on the outside.



One way light can scatter from a spherical raindrop.

3.2 Consider a particle constrained to move on the surface described in cylindrical coordinates by $z = \alpha r^3$, subject to a constant gravitational force $\vec{F} = -mg\hat{e}_z$. Find the Lagrangian, two conserved quantities, and reduce the problem to a one dimensional problem. What is the condition for circular motion at constant r?

3.3 From the general expression for ϕ as an integral over r, applied to a three dimensional symmetrical harmonic oscillator $V(\vec{r}) = \frac{1}{2}kr^2$, integrate the equation, and show that the motion is an ellipse, with the center of force at the center of the ellipse. Consider the three complex quantities $Q_i = p_i - i\sqrt{km}r_i$, and show that each has a very simple equation of motion, as a consequence of which the nine quantities $Q_i^* Q_k$ are conserved. Identify as many as possible of these with previously known conserved quantities.

3.4 Show that if a particle under the influence of a central force has an orbit which is a circle passing *through* the point of attraction, then the force is a power law with $|F| \propto r^{-5}$. Assuming the potential is defined so that $U(\infty) = 0$, show that for this particular orbit $E = 0$, find the period, and by expressing $\dot{x}$, $\dot{y}$ and the speed as a function of the angle measured from the center of the circle, and its derivative, show that $\dot{x}$, $\dot{y}$ and the speed all go to infinity as the particle passes through the center of force.

Chapter 4

Rigid Body Motion

In this chapter we develop the dynamics of a rigid body, one in which all interparticle distances are fixed by internal forces of constraint. This is, of course, an idealization which ignores elastic and plastic deformations to which any real body is susceptible, but it is an excellent approximation for many situations, and vastly simplifies the dynamics of the very large number of constituent particles of which any macroscopic body is made. In fact, it reduces the problem to one with six degrees of freedom. While the ensuing motion can still be quite complex, it is tractible. In the process we will be dealing with a configuration space which is a group, and is not a Euclidean space. Degrees of freedom which lie on a group manifold rather than Euclidean space arise often in applications in quantum mechanics and quantum field theory, in addition to the classical problems we will consider such as gyroscopes and tops.

4.1 Configuration space for a rigid body

A macroscopic body is made up of a very large number of atoms. Describing the motion of such a system without some simplifications is clearly impossible. Many objects of interest, however, are very well approximated by the assumption that the distances between the atoms

in the body are fixed[1],

$$|\vec{r}_\alpha - \vec{r}_\beta| = c_{\alpha\beta} = \text{ constant.} \tag{4.1}$$

This constitutes a set of holonomic constraints, but not independent ones, as we have here $\frac{1}{2}n(n-1)$ constraints on $3n$ coordinates. Rather than trying to solve the constraints, we can understand what are the generalized coordinates by recognizing that the possible motions which leave the interparticle lengths fixed are combinations of

- translations of the body as a whole, $\vec{r}_\alpha \to \vec{r}_\alpha + \vec{C}$,
- rotations of the body about some fixed, or "marked", point.

We will need to discuss how to represent the latter part of the configuration, (including what a rotation is), and how to reexpress the kinetic and potential energies in terms of this configuration space and its velocities.

The first part of the configuration, describing the translation, can be specified by giving the coordinates of the marked point fixed in the body, $\widetilde{R}(t)$. Often, but not always, we will choose this marked point to be the center of mass $\vec{R}(t)$ of the body. In order to discuss other points which are part of the body, we will use an orthonormal coordinate system fixed in the body, known as the **body coordinates**, with the origin at the fixed point $\widetilde{R}$. The constraints mean that the position of each particle of the body has fixed coordinates in terms of this coordinate system. Thus the dynamical configuration of the body is completely specified by giving the orientation of these coordinate axes in addition to $\widetilde{R}$. This orientation needs to be described relative to a fixed inertial coordinate system, or **inertial coordinates**, with orthonormal basis $\hat{e}_i$.

Let the three orthogonal unit vectors defining the body coordinates be $\hat{e}'_i$, for $i = 1, 2, 3$. Then the position of any particle α in the body which has coordinates $b'_{\alpha i}$ in the body coordinate system is at the position $\vec{r}_\alpha = \widetilde{R} + \sum_i b'_{\alpha i}\hat{e}'_i$. In order to know its components in the

[1] In this chapter we will use Greek letters as subscripts to represent the different particles within the body, reserving Latin subscripts to represent the three spatial directions.

inertial frame $\vec{r}_\alpha = \sum_i r_{\alpha i}\hat{e}_i$ we need to know the coordinates of the three vectors $\hat{e}'_i$ in terms of the inertial coordinates,

$$\hat{e}'_i = \sum_j A_{ij}\hat{e}_j. \tag{4.2}$$

The nine quantities A_{ij}, together with the three components of $\widetilde{R} = \sum \widetilde{R}_i\hat{e}_i$, specify the position of every particle,

$$r_{\alpha i} = \tilde{R}_i + \sum_j b'_{\alpha j}A_{ji},$$

and the configuration of the system is completely specified by $\widetilde{R}_i(t)$ and $A_{ij}(t)$.

The nine real quantities in the matrix A_{ij} are not independent, for the basis vectors $\hat{e}'_i$ of the body-fixed coordinate system are orthonormal,

$$\hat{e}'_i \cdot \hat{e}'_k = \delta_{ik} = \sum_{j\ell} A_{ij}A_{k\ell}\hat{e}_j \cdot \hat{e}_\ell = \sum_{j\ell} A_{ij}A_{k\ell}\delta_{j\ell} = \sum_j A_{ij}A_{kj},$$

or in matrix languag $AA^T = \mathbb{1}$. Such a matrix , whose transpose is equal to its inverse, is called **orthogonal**, and is a transformation of basis vectors which preserves orthonormality of the basis vectors. Because they play such an important role in the study of rigid body motion, we need to explore the properties of orthogonal transformations in some detail.

4.1.1 Orthogonal Transformations

There are two ways of thinking about an orthogonal transformation A and its action on an orthonormal basis, (Eq. 4.2). One way is to consider that $\{\hat{e}_i\}$ and $\{\hat{e}'_i\}$ are simply different basis vectors used to describe the same physical vectors in the same vector space. A vector $\vec{V}$ is the same vector whether it is expanded in one basis $\vec{V} = \sum_j V_j\hat{e}_j$ or the other $\vec{V} = \sum_i V'_i\hat{e}'_i$. Thus

$$\vec{V} = \sum_j V_j\hat{e}_j = \sum_i V'_i\hat{e}'_i = \sum_{ij} V'_i A_{ij}\hat{e}_j,$$

and we may conclude from the fact that the $\hat{e}_j$ are linearly independent that $V_j = \sum_i V_i' A_{ij}$, or in matrix notation that $V = A^T V'$. Because A is orthogonal, multiplying by A (from the left) gives $V' = AV$, or

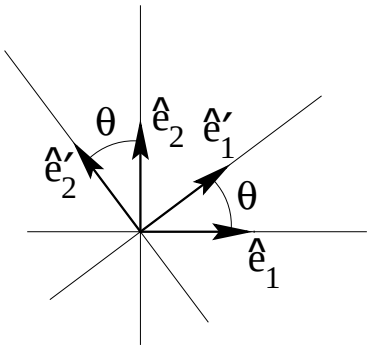
$$V_i' = \sum_j A_{ij} V_j. \tag{4.3}$$

Thus A is to be viewed as a rule for giving the primed basis vectors in terms of the unprimed ones (4.2), and also for giving the components of a vector in the primed coordinate system in terms of the components in the unprimed one (4.3). This picture of the role of A is called the **passive** interpretation.

One may also use matrices to represent a real physical transformation of an object or quantity. In particular, Eq. 4.2 gives A the interpretation of an operator that rotates each of the coordinate basis $\hat{e}_1, \hat{e}_2, \hat{e}_3$ into the corresponding new vector $\hat{e}_1'$, $\hat{e}_2'$, or $\hat{e}_3'$. For real rotation of the physical system, all the vectors describing the objects are changed by the rotation into new vectors $\vec{V} \to \vec{V}^{(R)}$, physically different from the original vector, but having the same coordinates in the primed basis as V has in the unprimed basis. This is called the **active** interpretation of the transformation. Both active and passive views of the transformation apply here, and this can easily lead to confusion. The transformation $A(t)$ is the physical transformation which rotated the body from some standard orientation, in which the body axes $\hat{e}_i'$ were parallel to the "lab frame" axes $\hat{e}_i$, to the configuration of the body at time t. But it also gives the relation of the components of the same position vectors (at time t) expressed in body fixed and lab frame coordinates.

If we first consider rotations in two dimensions, it is clear that they are generally described by the counterclockwise angle θ through which the basis is rotated,

$$\begin{aligned} \hat{e}'_1 &= \cos\theta\hat{e}_1 + \sin\theta\hat{e}_2 \\ \hat{e}'_2 &= -\sin\theta\hat{e}_1 + \cos\theta\hat{e}_2 \end{aligned}$$



corresponding to the matrix

$$A = \begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix}. \qquad (4.4)$$

Clearly taking the transpose simply changes the sign of θ, which is just what is necessary to produce the inverse transformation. Thus each two dimensional rotation is an orthogonal transformation. The orthogonality equation $A \cdot A^{-1} = 1$ has four matrix elements. It is straightforward to show that these four equations on the four elements of A determine A to be of the form 4.4 except that the sign of the bottom row is undetermined. For example, the transformation $\hat{e}'_1 = \hat{e}_1$, $\hat{e}'_2 = -\hat{e}_2$ is orthogonal but is not a rotation. Let us call this transformation P. Thus any two-dimensional orthogonal matrix is a rotation or is P followed by a rotation. The set of all real orthogonal matrices in two dimensions is called $O(2)$, and the subset consisting of rotations is called $SO(2)$.

In three dimensions we need to take some care with what we mean by a rotation. On the one hand, we might mean that the transformation has some fixed axis and is a rotation through some angle about that axis. Let us call that a **rotation about an axis**. On the other hand, we might mean all transformations we can produce by a sequence of rotations about various axes. Let us define **rotation** in this sense. Clearly if we consider the rotation R which rotates the basis $\{\hat{e}\}$ into the basis $\{\hat{e}'\}$, and if we have another rotation R' which rotates $\{\hat{e}'\}$ into $\{\hat{e}''\}$, then the transformation which first does R and then does R', called the **composition** of them, $\breve{R} = R' \circ R$, is also a rotation in this latter sense. As $\hat{e}''_i = \sum_j R'_{ij}\hat{e}'_j = \sum_{ij} R'_{ij}R_{jk}\hat{e}_k$, we see that $\breve{R}_{ik} = \sum_j R'_{ij}R_{jk}$ and $\hat{e}''_i = \sum_k \breve{R}_{ik}\hat{e}_k$. Thus the composition $\breve{R} = R'R$ is given by matrix multiplication. In two dimensions, straightforward evaluation will verify that if R and R' are of the form (4.4) with angles θ and θ' respectively, the product $\breve{R}$ is of the same form with angle $\breve{\theta} = \theta+\theta'$. Thus all rotations are rotations about an axis there. Rotations in

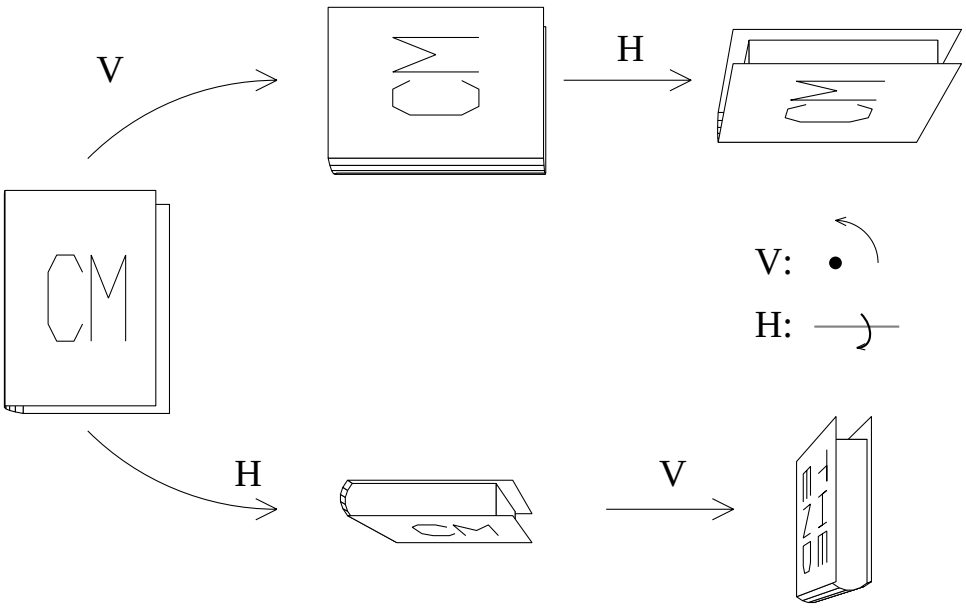


Figure 4.1: The results of applying the two rotations H and V to a book depends on which is done first. Thus rotations do not commute. Here we are looking down at a book which is originally lying face up on a table. V is a rotation about the vertical z-axis, and H is a rotation about a fixed axis pointing to the right, each through 90°.

three dimensions are a bit more complex, because they can take place in different directions as well as through different angles. We can still represent the composition of rotations with matrix multiplication, now of 3×3 matrices. In general, matrices do not commute, $AB \neq BA$, and this is indeed reflected in the fact that the effect of performing two rotations depends in the order in which they are done. A graphic illustration is worth trying. Let V be the process of rotating an object through 90° about the vertical z-axis, and H be a rotation through 90° about the x-axis, which goes goes off to our right. If we start with the book lying face up facing us on the table, and first apply V and then H, we wind up with the binding down and the front of the book facing us. If, however, we start from the same position but apply first H and then V, we wind up with the book standing upright on the table with the binding towards us. Clearly the operations H and V do not commute.

It is clear that any composition of rotations must be orthogonal, as any set of orthonormal basis vectors will remain orthonormal under each transformation. It is also clear that there is a three dimensional version of P, say $\hat{e}'_1 = \hat{e}_1$, $\hat{e}'_2 = \hat{e}_2$, $\hat{e}'_3 = -\hat{e}_3$, which is orthogonal but not a composition of rotations, for it changes a right-handed coordinate system (with $\hat{e}_1 \times \hat{e}_2 = \hat{e}_3$) to a left handed one, while rotations preserve the handedness. It is straightforward to show that any composition of orthogonal matrices is orthogonal, for if $AA^T = \mathbb{1}$ and $BB^T = \mathbb{1}$ and $C = AB$, then $CC^T = AB(AB)^T = ABB^TA^T = A\,\mathbb{1}\,A^T = \mathbb{1}$, and C is orthogonal as well. So the rotations are a subset of the set $O(N)$ of orthogonal matrices.

4.1.2 Groups

This set of orthogonal matrices is a group, which means that the set $O(N)$ satisfies the following requirements, which we state for a general set G.

A set G of elements $A, B, C, ...$ together with a **group multiplication** rule ($\odot$) for combining two of them, is a **group** if

- *Given any two elements A and B in the group, the product $A \odot B$ is also in the group.* One then says that the set G is **closed under** $\odot$. In our case the group multiplication is ordinary matrix multiplication, the group consists of all 3×3 orthogonal real matrices, and we have just shown that it is closed.

- *The product rule is* **associative***; for every $A, B, C \in G$, we have $A \odot (B \odot C) = (A \odot B) \odot C$.* For matrix multiplication this is simply due to the commutivity of finite sums, $\sum_i \sum_j = \sum_j \sum_i$.

- *There is an element e in G, called the identity, such that for every element $A \in G$, $eA = Ae = A$.* In our case e is the unit matrix $\mathbb{1}$, $\mathbb{1}_{ij} = \delta_{ij}$.

- *Every element $A \in G$ has an element $A^{-1} \in G$ such that $AA^{-1} = A^{-1}A = e$.* This element is called the inverse of A, and in the case of orthogonal matrices is the inverse matrix, which always exists, because for orthogonal matrices the inverse is the transpose, which always exists for any matrix.

While the constraints 4.1 would permit $A(t)$ to be any orthogonal matrix, the nature of Newtonian mechanics requires it to vary continuously in time. If the system starts with $A = \mathbb{1}$, there must be a continuous path in the space of orthogonal matrices to the configuration $A(t)$ at any later time. But the set of matrices $O(3)$ is not connected in this fashion: there is no path from $A = \mathbb{1}$ to $A = P$. To see it is true, we look at the determinant of A. From $AA^T = \mathbb{1}$ we see that $\det(AA^T) = 1 = \det(A)\det(A^T) = (\det A)^2$ so $\det A = \pm 1$ for all orthogonal matrices A. But the determinant varies continuously as the matrix does, so no continuous variation of the matrix can lead to a jump in its determinant. Thus the matrices which represent rotations have unit determinant, $\det A = +1$, and are called **unimodular**.

The set of all unimodular orthogonal matrices in N dimensions is called $SO(N)$. It is a subset of $O(N)$, the set of all orthogonal matrices in N dimensions. Clearly all rotations are in this subset. The subset is closed under multiplication, and the identity and the inverses of elements in $SO(N)$ are also in $SO(N)$, for their determinants are clearly 1. Thus $SO(N)$ is a **subgroup** of $O(N)$. It is actually the set of rotations, but we shall prove this statement only for the case $N = 3$, which is the immediately relevant one. Simultaneously we will show that every rotation in three dimensions is a rotation about an axis. We have already proven it for $N = 2$. We now show that every $A \in SO(3)$ has one vector it leaves unchanged or invariant, so that it is effectively a rotation in the plane perpendicular to this direction, or in other words a rotation about the axis it leaves invariant. The fact that every unimodular orthogonal matrix in three dimensions is a rotation about an axis is known as **Euler's Theorem**. To show that it is true, we note that if A is orthogonal and has determinant 1,

$$\begin{aligned}\det\left\{(A-\mathbb{1})A^T\right\} &= \det(\mathbb{1}-A^T) = \det(\mathbb{1}-A)\\ &= \det(A-\mathbb{1})\det(A) = \det(-(\mathbb{1}-A)) = (-1)^3\det(\mathbb{1}-A)\\ &= -\det(\mathbb{1}-A),\end{aligned}$$

so $\det(\mathbb{1} - A) = 0$ and $\mathbb{1} - A$ is a singular matrix. Then there exists a vector $\vec{\omega}$ which is annihilated by it, $(\mathbb{1} - A)\vec{\omega} = 0$, or $A\vec{\omega} = \vec{\omega}$, and $\vec{\omega}$ is invariant under A. Of course this determines only the direction of $\vec{\omega}$, and only up to sign. If we choose a new coordinate system in which

the $\tilde{z}$-axis points along $\vec{\omega}$, we see that the elements $\tilde{A}_{i3} = (0, 0, 1)$, and orthogonality gives $\sum A_{3j}^2 = 1 = A_{33}^2$ so $A_{31} = A_{32} = 0$. Thus A is of the form

$$A = \begin{pmatrix} & (\,B\,) & & 0 \\ & & & 0 \\ 0 & 0 & & 1 \end{pmatrix}$$

where B is an orthogonal unimodular 2×2 matrix, which is therefore a rotation about the z-axis through some angle ω, which we may choose to be in the range $\omega \in (-\pi, \pi]$. It is natural to define the vector $\vec{\omega}$, whose direction only was determined above, to be $\vec{\omega} = \omega \hat{e}_{\tilde{z}}$. Thus we see that the set of orthogonal unimodular matrices is the set of rotations, and elements of this set may be specified by a vector[2] of length $\leq \pi$.

Thus we see that the rotation which determines the orientation of a rigid body can be described by the three degrees of freedom $\vec{\omega}$. Together with the translational coordinates $\widetilde{R}$, this parameterizes the configuration space of the rigid body, which is six dimensional. It is important to recognize that this is not motion in a flat six dimensional configuration space, however. For example, the configurations with $\vec{\omega} = (0, 0, \pi - \epsilon)$ and $\vec{\omega} = (0, 0, -\pi + \epsilon)$ approach each other as $\epsilon \to 0$, so that motion need not even be continuous in $\vec{\omega}$. The composition of rotations is by multiplication of the matrices, *not* by addition of the $\vec{\omega}$'s. There are other ways of describing the configuration space, two of which are known as Euler angles and Cayley-Klein parameters, but none of these make describing the space very intuitive. For some purposes we do not need all of the complications involved in describing finite rotations, but only what is necessary to describe infinitesimal changes between the configuration at time t and at time $t + \Delta t$. We will discuss these applications first. Later, when we do need to discuss the configuration in section 4.4.2, we will define Euler angles.

[2]More precisely, we choose $\vec{\omega}$ along one of the two opposite directions left invariant by A, so that the the angle of rotation is non-negative and $\leq \pi$. This specifies a point in or on the surface of a three dimensional ball of radius π, but in the case when the angle is exactly π the two diametrically opposed points both describe the same rotation. Mathematicians say that the space of $SO(3)$ is three-dimensional real projective space $P_3(\mathbb{R})$.

4.2 Kinematics in a rotating coordinate system

We have seen that the rotations form a group. Let us describe the configuration of the body coordinate system by the position $\widetilde{R}(t)$ of a given point and the rotation matrix $A(t) : \hat{e}_i \to \hat{e}'_i$ which transforms the canonical fixed basis (inertial frame) into the body basis. A given particle of the body is fixed in the body coordinates, but this, of course, is not an inertial coordinate system, but a rotating and possibly accelerating one. We need to discuss the transformation of kinematics between these two frames. While our current interest is in rigid bodies, we will first derive a general formula for rotating (and accelerating) coordinate systems.

Suppose a particle has coordinates $\vec{b}(t) = \sum_i b'_i(t)\hat{e}'_i(t)$ in the body system. We are not assuming at the moment that the particle is part of the rigid body, in which case the $b'_i(t)$ would be independent of time. In the inertial coordinates the particle has its position given by $\vec{r}(t) = \widetilde{R}(t) + \vec{b}(t)$, but the coordinates of $\vec{b}(t)$ are different in the space and body coordinates. Thus

$$r_i(t) = \widetilde{R}_i(t) + b_i(t) = \widetilde{R}_i(t) + \sum_j \left(A^{-1}(t)\right)_{ij} b'_j(t).$$

The velocity is $\vec{v} = \sum_i \dot{r}_i \hat{e}_i$, because the $\hat{e}_i$ are inertial and therefore considered stationary, so

$$\vec{v} = \dot{\widetilde{R}} + \sum_{ij} \left[\left(\frac{d}{dt} A^{-1}(t) \right)_{ij} b'_j(t) + \left(A^{-1}(t)\right)_{ij} \frac{db'_j(t)}{dt} \right] \hat{e}_i,$$

and *not* $\dot{\widetilde{R}} + \sum_i (db'_i/dt)\hat{e}'_i$, because the $\hat{e}'_i$ are themselves changing with time. We might define a "body time derivative"

$$\left(\dot{\vec{b}}\right)_b := \left(\frac{d}{dt}\vec{b}\right)_b := \sum_i \left(\frac{db'_i}{dt}\right) \hat{e}'_i,$$

but it is *not* the velocity of the particle α, even with respect to $\widetilde{R}(t)$, in the sense that physically a vector is basis independent, and its derivative

requires a notion of which basis vectors are considered time independent (inertial) and which are not. Converting the inertial evaluation to the body frame requires the velocity to include the dA^{-1}/dt term as well as the $\left(\dot{\vec{b}}\right)_b$ term.

What is the meaning of this extra term

$$\mathcal{V} = \sum_{ij} \left(\frac{d}{dt} A^{-1}(t)\right)_{ij} b'_j(t)\hat{e}_i \quad ?$$

The derivative is, of course,

$$\mathcal{V} = \lim_{\Delta t \to 0} \frac{1}{\Delta t} \sum_{ij} \left[A^{-1}(t+\Delta t)_{ij} - A^{-1}(t)_{ij}\right] b'_j(t)\hat{e}_i.$$

This expression has coordinates in the body frame with basis vectors from the inertial frame. It is better to describe it in terms of the body coordinates and body basis vectors by inserting $\hat{e}_i = \sum_k (A^{-1}(t)_{ik}\hat{e}'_k(t) = \sum_k A_{ki}(t)\hat{e}'_k(t)$. Then we have

$$\mathcal{V} = \sum_{kj} \hat{e}'_k \lim_{\Delta t \to 0} \frac{1}{\Delta t} \left[A(t)A^{-1}(t+\Delta t) - A(t)A^{-1}(t)\right]_{kj} b'_j(t).$$

The second term is easy enough to understand, as $A(t)A^{-1}(t) = \mathbb{1}$, so the full second term is just $\vec{b}$ expressed in the body frame. The interpretation of the first term is suggested by its matrix form: $A^{-1}(t+\Delta t)$ maps the body basis at $t+\Delta t$ to the inertial frame, and $A(t)$ maps this to the body basis at t. So together this is the infinitesimal rotation $\hat{e}'_i(t+\Delta t) \to \hat{e}'_i(t)$. This transformation must be close to an identity, as $\Delta t \to 0$. Let us expand it:

$$B := A(t)A^{-1}(t+\Delta t) = \mathbb{1} - \Omega'\Delta t + \mathcal{O}(\Delta t)^2. \tag{4.5}$$

Here Ω' is a matrix which has fixed (finite) elements as $\Delta t \to 0$, and is called the **generator** of the rotation. Note $B^{-1} = \mathbb{1} + \Omega'\Delta t$ to the order we are working, while the transpose $B^T = \mathbb{1} - \Omega'^T\Delta t$, so because we know B is orthogonal we must have that Ω' is **antisymmetric**, $\Omega' = -\Omega'^T$, $\Omega'_{ij} = -\Omega'_{ji}$.

Subtracting $\mathbb{1}$ from both sides of (4.5) and taking the limit shows that the matrix

$$\Omega'(t) = -A(t) \cdot \frac{d}{dt} A^{-1}(t) = \left(\frac{d}{dt} A(t) \right) \cdot A^{-1}(t),$$

where the latter equality follows from differentiating $A \cdot A^{-1} = \mathbb{1}$. The antisymmetric matrix Ω' is effectively a vector. Define $\omega'_k = \frac{1}{2} \sum_{ij} \epsilon_{kij} \Omega'_{ij}$. Then the ω'_k also determine the Ω'_{ij}:

$$\begin{aligned} \sum_k \epsilon_{ijk} \omega'_k &= \frac{1}{2} \sum_{k\ell m} \epsilon_{ijk} \epsilon_{k\ell m} \Omega'_{\ell m} \\ &= \frac{1}{2} \sum_{\ell m} \left(\delta_{i\ell} \delta_{jm} - \delta_{im} \delta_{j\ell} \right) \Omega'_{\ell m} = \frac{1}{2} (\Omega'_{ij} - \Omega'_{ji}) = \Omega'_{ij}, \end{aligned}$$

so ω'_k and Ω'_{ij} are essentially the same thing.

We have still not answered the question, "what is $\mathcal{V}$?"

$$\begin{aligned} \mathcal{V} &= \sum_{kj} \hat{e}'_k \lim_{\Delta t \to 0} \frac{1}{\Delta t} \left[B - \mathbb{1} \right]_{kj} b'_j = - \sum_{kj} \hat{e}'_k \Omega'_{kj} b'_j = - \sum_{kj\ell} \hat{e}'_k \epsilon_{kj\ell} \omega'_\ell b'_j \\ &= \vec{\omega} \times \vec{b}, \end{aligned}$$

where $\vec{\omega} = \sum_\ell \omega'_\ell \hat{e}'_\ell$. Thus we see that

$$\vec{v} = \dot{\vec{R}} + \vec{\omega} \times \vec{b} + (\dot{\vec{b}})_b, \tag{4.6}$$

and the second term, coming from $\mathcal{V}$, represents the motion due to the rotating coordinate system.

When differentiating a true vector, which is independent of the origin of the coordinate system, rather than a position, the first term in (4.6) is absent, so in general for a vector $\vec{C}$,

$$\frac{d}{dt} \vec{C} = \left(\frac{d\vec{C}}{dt} \right)_b + \omega \times \vec{C}. \tag{4.7}$$

The velocity $\vec{v}$ is a vector, as are $\dot{\vec{R}}$ and $\vec{b}$, the latter because it is the difference of two positions. The angular velocity $\vec{\omega}$ is also a vector, and its derivative is particularly simple, because

$$\dot{\vec{\omega}} = \frac{d}{dt} \vec{\omega} = \left(\frac{d\vec{\omega}}{dt} \right)_b + \vec{\omega} \times \vec{\omega} = \left(\frac{d\vec{\omega}}{dt} \right)_b. \tag{4.8}$$

Another way to understand (4.7) is as a simple application of Leibnitz' rule to $\vec{C} = \sum C'_i \hat{e}'_i$, noting that

$$\frac{d}{dt}\hat{e}'_i(t) = \sum_j \frac{d}{dt} A_{ij}(t)\hat{e}_j = \sum_j (\Omega' A)_{ij}\, \hat{e}_j = \sum_k \Omega'_{ik}\hat{e}'_k,$$

which means that the second term from Leibnitz is

$$\sum C'_i \frac{d}{dt}\hat{e}'_i(t) = \sum_{ik} C'_i \Omega'_{ik}\hat{e}'_k = \sum_{ijk} C'_i \epsilon_{ikj}\omega'_j \hat{e}'_k = \vec{\omega} \times \vec{C},$$

as given in (4.7). This shows that even the peculiar object $(\dot{\vec{b}})_b$ obeys (4.7).

Applying this to the velocity itself (4.6), we find the acceleration

$$\begin{aligned}
\vec{a} &= \frac{d}{dt}\vec{v} = \frac{d}{dt}\dot{\vec{R}} + \frac{d\omega}{dt} \times \vec{b} + \omega \times \frac{d}{dt}\vec{b} + \frac{d}{dt}(\dot{\vec{b}})_b \\
&= \ddot{\vec{R}} + \dot{\vec{\omega}} \times \vec{b} + \omega \times \left[\left(\frac{d\vec{b}}{dt} \right)_b + \vec{\omega} \times \vec{b} \right] + \left(\frac{d^2\vec{b}}{dt^2} \right)_b + \omega \times \left(\frac{d\vec{b}}{dt} \right)_b \\
&= \ddot{\vec{R}} + \left(\frac{d^2\vec{b}}{dt^2} \right)_b + 2\omega \times \left(\frac{d\vec{b}}{dt} \right)_b + \dot{\vec{\omega}} \times \vec{b} + \vec{\omega} \times \left(\omega \times \vec{b} \right).
\end{aligned}$$

This is a general relation between any orthonormal coordinate system and an inertial one, and in general can be used to describe physics in noninertial coordinates, regardless of whether that coordinate system is imbedded in a rigid body. The full force on the particle is $\vec{F} = m\vec{a}$, but if we use $\vec{r}$, $\vec{v}'$, and $\vec{a}'$ to represent $\vec{b}$, $(d\vec{b}/dt)_b$ and $(d^2\vec{b}/dt^2)_b$ respectively, we have an expression for the apparent force

$$m\vec{a}' = \vec{F} - m\ddot{\vec{R}} - 2m\vec{\omega} \times \vec{v}' - m\dot{\vec{\omega}} \times \vec{r} - m\vec{\omega} \times (\vec{\omega} \times \vec{r}).$$

The additions to the real force are the pseudoforce for an accelerating reference frame $-m\ddot{\vec{R}}$, the Coriolus force $-2m\vec{\omega} \times \vec{v}'$, an unnamed force involving the angular acceleration of the coordinate system $-m\dot{\vec{\omega}} \times \vec{r}$, and the centrifugal force $-m\vec{\omega} \times (\vec{\omega} \times \vec{r})$ respectively.

4.3 The moment of inertia tensor

Let us return to a rigid body, where the particles are constrained to keep the distances between them constant. Then the coordinates $b'_{\alpha i}$ in the body frame are independant of time, and

$$\vec{v}_\alpha = \dot{\widetilde{R}} + \omega \times \vec{b}_\alpha$$

so the individual momenta and the total momentum are

$$\begin{aligned} \vec{p}_\alpha &= m_\alpha \widetilde{V} + m_\alpha \vec{\omega} \times \vec{b}_\alpha \\ \vec{P} &= M\widetilde{V} + \vec{\omega} \times \sum_\alpha m_\alpha \vec{b}_\alpha \\ &= M\widetilde{V} + M\vec{\omega} \times \vec{B} \end{aligned}$$

where $\vec{B}$ is the center of mass position relative to the marked point $\widetilde{R}$.

4.3.1 Motion about a fixed point

Angular Momentum

We next evaluate the total angular momentum, $\vec{L} = \sum_\alpha \vec{r}_\alpha \times p_\alpha$. We will first consider the special case in which the body is rotating about the origin, so $\widetilde{R} \equiv 0$, and then we will return to the general case. As $\vec{p}_\alpha = m_\alpha \vec{\omega} \times \vec{b}_\alpha$ already involves a cross product, we will find a triple product, and will use the reduction formula[3]

$$\vec{A} \times \left(\vec{B} \times \vec{C}\right) = \vec{B}\left(\vec{A} \cdot \vec{C}\right) - \vec{C}\left(\vec{A} \cdot \vec{B}\right).$$

Thus

$$\begin{aligned} \vec{L} &= \sum_\alpha m_\alpha \vec{b}_\alpha \times \left(\vec{\omega} \times \vec{b}_\alpha\right) && (4.9) \\ &= \vec{\omega} \sum_\alpha m_\alpha \vec{b}_\alpha^2 - \sum_\alpha m_\alpha \vec{b}_\alpha \left(\vec{b}_\alpha \cdot \vec{\omega}\right). && (4.10) \end{aligned}$$

We see that, in general, $\vec{L}$ need not be parallel to the angular velocity $\vec{\omega}$, but it is always linear in $\vec{\omega}$. Thus it is possible to generalize the equation

[3]This formula is colloquially known as the **bac-cab** formula. It is proven in Appendix A.

$\vec{L} = I\vec{\omega}$ of elementary physics courses, but we need to generalize I from a multiplicative number to a linear operator which maps vectors into vectors, not necessarily in the same direction. In component language this linear operation is clearly in the form $L_i = \sum_j I_{ij}\omega_j$, so I is a 3×3 matrix. Rewriting (4.10), we have

$$\begin{aligned} L_i &= \omega_i \sum_\alpha m_\alpha \vec{b}_\alpha^2 - \sum_\alpha m_\alpha b_{\alpha i} \left(\vec{b}_\alpha \cdot \vec{\omega}\right). \\ &= \sum_j \sum_\alpha m_\alpha \left(\vec{b}_\alpha^2 \delta_{ij} - b_{\alpha i} b_{\alpha j}\right) \omega_j \\ &\equiv \sum_j I_{ij}\omega_j, \end{aligned}$$

where

$$I_{ij} = \sum_\alpha m_\alpha \left(\vec{b}_\alpha^2 \delta_{ij} - b_{\alpha i} b_{\alpha j}\right)$$

is the **inertia tensor** about the fixed point $\widetilde{R}$. In matrix form, we now have (4.10) as

$$\vec{L} = I \cdot \vec{\omega}, \tag{4.11}$$

where $I \cdot \vec{\omega}$ means a vector with components $(I \cdot \vec{\omega})_i = \sum_j I_{ij}\omega_j$.

If we consider the rigid body in the continuum limit, the sum over particles becomes an integral over space times the density of matter,

$$I_{ij} = \int d^3 b \rho(\vec{b}) \left(\vec{b}^2 \delta_{ij} - b_i b_j\right). \tag{4.12}$$

Kinetic energy

For a body rotating about a fixed point $\tilde{R}$,

$$T = \frac{1}{2}\sum_\alpha m_\alpha \vec{v}_\alpha^2 = \frac{1}{2}\sum_\alpha m_\alpha \left(\vec{\omega} \times \vec{b}_\alpha\right) \cdot \left(\vec{\omega} \times \vec{b}_\alpha\right).$$

From the general 3-dimensional identity[4]

$$\left(\vec{A} \times \vec{B}\right) \cdot \left(\vec{C} \times \vec{D}\right) = \vec{A} \cdot \vec{C}\vec{B} \cdot \vec{D} - \vec{A} \cdot \vec{D}\vec{B} \cdot \vec{C},$$

[4]See Appendix A for a hint on how to derive this.

we have

$$\begin{aligned} T &= \frac{1}{2}\sum_\alpha m_\alpha \left[\vec{\omega}^{\,2}\vec{b}_\alpha^{\,2} - \left(\vec{\omega}\cdot\vec{b}_\alpha\right)^2\right] \\ &= \frac{1}{2}\sum_{ij}\omega_i\omega_j \sum_\alpha m_\alpha\left(\vec{b}_\alpha^{\,2}\delta_{ij} - \vec{b}_{\alpha i}\vec{b}_{\alpha j}\right) \\ &= \frac{1}{2}\sum_{ij}\omega_i I_{ij}\omega_j. \end{aligned} \tag{4.13}$$

or

$$T = \frac{1}{2}\vec{\omega}\cdot I\cdot\vec{\omega}.$$

Noting that $\sum_j I_{ij}\omega_j = L_i$, $T = \frac{1}{2}\vec{\omega}\cdot\vec{L}$ for a rigid body rotating about the origin, with $\vec{L}$ measured from that origin.

4.3.2 More General Motion

When the marked point $\widetilde{R}$ is not fixed in space, there is nothing special about it, and we might ask whether it would be better to evaluate the moment of inertia about some other point. Working in the body-fixed coordinates, we may consider a given point $\vec{b}$ and evaluate the moment of inertia about that point, rather than about the origin. This means $\vec{b}_\alpha$ is replaced by $\vec{b}_\alpha - \vec{b}$, so

$$\begin{aligned} I_{ij}^{(\vec{b})} &= \sum_\alpha m_\alpha\left[\left(\vec{b}_\alpha - \vec{b}\right)^2\delta_{ij} - \left(b_{\alpha i} - b_i\right)\left(b_{\alpha j} - b_j\right)\right] \\ &= I_{ij}^{(0)} + M\left[\left(-2\vec{b}\cdot\vec{B} + b^2\right)\delta_{ij} + B_i b_j + b_i B_j - b_i b_j\right], \end{aligned} \tag{4.14}$$

where we recall that $\vec{B}$ is the position of the center of mass with respect to $\widetilde{R}$, the origin of the body fixed coordinates. Subtracting the moment of inertia about the center of mass, given by (4.14) with $b \to B$, we have

$$\begin{aligned} I_{ij}^{(\vec{b})} - I_{ij}^{(\vec{B})} &= M\left[\left(-2\vec{b}\cdot\vec{B} + b^2 + B^2\right)\delta_{ij} + B_i b_j + b_i B_j - b_i b_j - B_i B_j\right] \\ &= M\left[\left(\vec{b} - \vec{B}\right)^2\delta_{ij} - \left(b_i - B_i\right)\left(b_j - B_j\right)\right]. \end{aligned} \tag{4.15}$$

Note the difference is independent of the origin of the coordinate system, depending only on the vector $\breve{b} = \vec{b} - \vec{B}$.

A possible axis of rotation can be specified by a point $\vec{b}$ through which it passes, together with a unit vector $\hat{n}$ in the direction of the axis[5]. The **moment of inertia** about the axis $(\vec{b}, \hat{n})$ is defined as $\hat{n} \cdot I^{(\vec{b})} \cdot \hat{n}$. If we compare this to the moment about a parallel axis through the center of mass, we see that

$$\begin{aligned} \hat{n} \cdot I^{(\vec{b})} \cdot \hat{n} - \hat{n} \cdot I^{(\mathrm{cm})} \cdot \hat{n} &= M\left[\breve{b}^2 \hat{n}^2 - (\breve{b} \cdot \hat{n})^2\right] \\ &= M(\hat{n} \times \breve{b})^2 = M\breve{b}_\perp^2, \end{aligned} \tag{4.16}$$

where $\breve{b}_\perp$ is the projection of the vector, from the center of mass to $\vec{b}$, onto the plane perpendicular to the axis. Thus the moment of inertia about any axis is the moment of inertia about a parallel axis through the center of mass, plus $M\ell^2$, where $\ell = \breve{b}_\perp$ is the distance between these two axes. This is known as the **parallel axis theorem**.

The general motion of a rigid body involves both a rotation and a translation of a given point $\widetilde{R}$. Then

$$\dot{\vec{r}}_\alpha = \widetilde{V} + \vec{\omega} \times \vec{b}_\alpha, \tag{4.17}$$

where $\widetilde{V}$ and $\vec{\omega}$ may be functions of time, but they are the same for all particles α. Then the angular momentum about the *origin* is

$$\begin{aligned} \vec{L} &= \sum_\alpha m_\alpha \vec{r}_\alpha \times \dot{\vec{r}}_\alpha = \sum_\alpha m_\alpha \vec{r}_\alpha \times \widetilde{V} + \sum_\alpha m_\alpha \left(\widetilde{R} + \vec{b}_\alpha\right) \times \left(\vec{\omega} \times \vec{b}_\alpha\right) \\ &= M\vec{R} \times \widetilde{V} + I^{(0)} \cdot \vec{\omega} + M\widetilde{R} \times (\vec{\omega} \times \vec{B}), \end{aligned} \tag{4.18}$$

where the inertia tensor $I^{(0)}$ is still measured about $\widetilde{R}$, even though that is not a fixed point. Recall that $\vec{R}$ is the laboratory position of the center of mass, while $\vec{B}$ is its position in the body-fixed system. The kinetic energy is now

$$T = \sum_\alpha \frac{1}{2} m_\alpha \dot{\vec{r}}_\alpha^{\,2} = \frac{1}{2} \sum_\alpha m_\alpha \left(\widetilde{V} + \vec{\omega} \times \vec{b}_\alpha\right) \cdot \left(\widetilde{V} + \vec{\omega} \times \vec{b}_\alpha\right)$$

[5]Actually, this gives more information than is needed to specify an axis, as $\vec{b}$ and $\vec{b}'$ specify the same axis if $\vec{b} - \vec{b}' \propto \hat{n}$. In the expression for the moment of inertia about the axis, (4.16), we see that the component of $\vec{b}$ parallel to $\hat{n}$ does not affect the result.

$$\begin{aligned} &= \frac{1}{2}\sum_\alpha m_\alpha \widetilde{V}^2 + \widetilde{V}\cdot\left(\vec{\omega}\times\sum_\alpha m_\alpha \vec{b}_\alpha\right) + \frac{1}{2}\sum_\alpha m_\alpha\left(\vec{\omega}\times\vec{b}_\alpha\right)^2 \\ &= \frac{1}{2}M\widetilde{V}^2 + M\widetilde{V}\cdot\left(\vec{\omega}\times\vec{B}\right) + \frac{1}{2}\vec{\omega}\cdot I^{(0)}\cdot\vec{\omega} \end{aligned} \tag{4.19}$$

and again the inertia tensor is calculated about the arbitrary point $\widetilde{R}$. We will see that it makes more sense to use the center of mass.

Simplification Using the Center of Mass

As each $\dot{\vec{r}}_\alpha = \widetilde{V} + \vec{\omega}\times\vec{b}_\alpha$, the center of mass velocity is given by

$$M\vec{V} = \sum_\alpha m_\alpha \dot{\vec{r}}_\alpha = \sum_\alpha m_\alpha\left(\widetilde{V} + \vec{\omega}\times\vec{b}_\alpha\right) = M\left(\widetilde{V} + \vec{\omega}\times\vec{B}\right), \tag{4.20}$$

so $\frac{1}{2}M\vec{V}^{\,2} = \frac{1}{2}M\widetilde{V}^2 + M\widetilde{V}\cdot(\vec{\omega}\times\vec{B}) + \frac{1}{2}M(\omega\times\vec{B})^2$. Comparing with 4.19, we see that

$$T = \frac{1}{2}M\vec{V}^{\,2} - \frac{1}{2}M(\vec{\omega}\times\vec{B})^2 + \frac{1}{2}\vec{\omega}\cdot I^{(0)}\cdot\vec{\omega}.$$

The last two terms can be written in terms of the inertia tensor about the center of mass. From 4.15 with $\vec{b} = 0$ for $\widetilde{R} = \vec{R}$,

$$I_{ij}^{(cm)} = I_{ij}^{(0)} - MB^2\delta_{ij} + MB_iB_j.$$

Using the formula for $\left(\vec{A}\times\vec{B}\right)\cdot\left(\vec{C}\times\vec{D}\right)$ again,

$$\begin{aligned} T &= \frac{1}{2}M\vec{V}^{\,2} - \frac{1}{2}M\left[\vec{\omega}^2\vec{B}^2 - \left(\vec{\omega}\cdot\vec{B}\right)^2\right] + \frac{1}{2}\vec{\omega}\cdot I^{(0)}\cdot\vec{\omega} \\ &= \frac{1}{2}M\vec{V}^{\,2} + \frac{1}{2}\vec{\omega}\cdot I^{(cm)}\cdot\vec{\omega}. \end{aligned} \tag{4.21}$$

A similar expression holds for the angular momentum. Inserting $\widetilde{V} = \vec{V} - \vec{\omega}\times\vec{B}$ into (4.18),

$$\begin{aligned} \vec{L} &= M\vec{R}\times\left[\vec{V} - \vec{\omega}\times\vec{B}\right] + I^{(0)}\cdot\vec{\omega} + M\widetilde{R}\times(\vec{\omega}\times\vec{B}) \\ &= M\vec{R}\times\vec{V} - M(\vec{R} - \widetilde{R})\times(\vec{\omega}\times\vec{B}) + I^{(0)}\cdot\vec{\omega} \\ &= M\vec{R}\times\vec{V} - M\vec{B}\times(\vec{\omega}\times\vec{B}) + I^{(0)}\cdot\vec{\omega} \\ &= M\vec{R}\times\vec{V} - M\vec{\omega}\,B^2 + M\vec{B}\,\vec{\omega}\cdot\vec{B} + I^{(0)}\cdot\vec{\omega} \\ &= M\vec{R}\times\vec{V} + I^{(cm)}\cdot\vec{\omega}. \end{aligned} \tag{4.22}$$

These two decompositions, (4.21) and (4.22), have a reasonable interpretation: the total angular momentum is the angular momentum about the center of mass, plus the angular momentum that a point particle of mass M and position $\vec{R}(t)$ would have. Similiarly, the total kinetic energy is the rotational kinetic energy of the body rotating about its center of mass, plus the kinetic energy of the fictious point particle at the center of mass.

Note that if we go back to the situation where the marked point $\widetilde{R}$ is stationary at the origin of the lab coordinates, $\widetilde{V} = 0$, $\vec{L} = I \cdot \vec{\omega}$, $T = \frac{1}{2}\vec{\omega} \cdot I \cdot \vec{\omega} = \frac{1}{2}\vec{\omega} \cdot \vec{L}$.

The angular momentum in Eqs. 4.18 and 4.22 is the angular momentum measured about the origin of the lab coordinates, $\vec{L} = \sum_\alpha m_\alpha \vec{r}_\alpha \times v_\alpha$. It is useful to consider the angular momentum as measured about the center of mass,

$$\vec{L}^{\,\mathrm{cm}} = \sum_\alpha m_\alpha \left(\vec{r}_\alpha - \vec{R}\right) \times \left(\vec{v}_\alpha - \vec{V}\right) = \vec{L} - M\vec{r} \times \vec{V}, \qquad (4.23)$$

so we see that the angular momentum, measured about the center of mass, is just $I^{(cm)} \cdot \vec{\omega}$.

The parallel axis theorem is also of the form of a decomposition. The inertia tensor about a given point $\vec{r}$ given by (4.15) is

$$I_{ij}^{(r)} \;=\; I_{ij}^{(cm)} + M\left[\left(\vec{r} - \vec{R}\right)^2 \delta_{ij} - \left(r_i - R_i\right)\left(r_j - R_j\right)\right].$$

This is, once again, the sum of the quantity, here the inertia tensor, of the body about the center of mass, plus the value a particle of mass M at the center of mass $\vec{R}$ would have, evaluated about $\vec{r}$.

There is another theorem about moments of inertia, though much less general — it only applies to a planar object — let's say in the xy plane, so that $z_\alpha \approx 0$ for all the particles constituting the body. As

$$\begin{aligned} I_{zz} &= \sum_\alpha m_\alpha \left(x_\alpha^2 + y_\alpha^2\right) \\ I_{xx} &= \sum_\alpha m_\alpha \left(y_\alpha^2 + z_\alpha^2\right) = \sum_\alpha m_\alpha y_\alpha^2 \\ I_{yy} &= \sum_\alpha m_\alpha \left(x_\alpha^2 + z_\alpha^2\right) = \sum_\alpha m_\alpha x_\alpha^2, \end{aligned}$$

we see that $I_{zz} = I_{xx} + I_{yy}$, the moment of inertia about an axis perpendicular to the body is the sum of the moments about two perpendicular axes within the body, through the same point. This is known as the **perpendicular axis theorem**. As an example of its usefulness we calculate the moments for a thin uniform ring lying on the circle $x^2 + y^2 = R^2$, $z = 0$, about the origin. As every particle of the ring has the same distance R from the z-axis, the moment of inertia I_{zz} is simply MR^2. As $I_{xx} = I_{yy}$ by symmetry, and as the two must add up to I_{zz}, we have, by a simple indirect calculation, $I_{xx} = \frac{1}{2}MR^2$.

The parallel axis theorem (4.16) is also a useful calculational tool. Consider the moment of inertia of the ring about an axis parallel to its axis of symmetry but through a point on the ring. About the axis of symmetry, $I_{zz} = MR^2$, and $b_\perp = R$, so about a point on the ring, $I_{zz} = 2MR^2$. If instead, we want the moment about a tangent to the ring, $I_{xx} = I_{xx}^{(cm)} + MR^2 = \frac{1}{2}MR^2 + MR^2 = 3MR^2/2$. Of course for I_{yy} the $b_\perp = 0$, so $I_{yy} = \frac{1}{2}MR^2$, and we may verify that $I_{zz} = I_{xx} + I_{yy}$ about this point as well.

Principal axes

If an object has an axial symmetry about z, we may use cylindrical polar coordinates (ρ, θ, z). Then its density $\mu(\rho, \theta, z)$ must be independent of θ, and

$$\begin{aligned}
& I_{ij} &=& \int dz\, \rho d\rho\, d\theta\, \mu(\rho, z) \left[(\rho^2 + z^2)\delta_{ij} - r_i r_j\right], \\
\text{so} \quad & I_{xz} &=& \int dz\, \rho d\rho\, \mu(\rho, z) d\theta\, (-z\rho\cos\theta) = 0 \\
& I_{xy} &=& \int dz\, \rho d\rho\, \mu(\rho, z) d\theta\, (\rho^2 \sin\theta\cos\theta) = 0 \\
& I_{xx} &=& \int dz\, \rho d\rho\, \mu(\rho, z) d\theta\, \left[(\rho^2 + z^2 - \rho^2\cos^2\theta\right] \\
& I_{yy} &=& \int dz\, \rho d\rho\, \mu(\rho, z) d\theta\, \left[(\rho^2 + z^2 - \rho^2\sin^2\theta\right] \;=\; I_{xx}
\end{aligned}$$

Thus the inertia tensor is diagonal and has two equal elements,

$$I_{ij} = \begin{pmatrix} I_{xx} & 0 & 0 \\ 0 & I_{xx} & 0 \\ 0 & 0 & I_{zz} \end{pmatrix}.$$

In general, an object need not have an axis of symmetry, and even a diagonal inertia tensor need not have two equal "eigenvalues". Even if a body has no symmetry, however, there is always a choice of axes, a coordinate system, such that in this system the inertia tensor is diagonal. This is because I_{ij} is always a real symmetric tensor, and any such tensor can be brought to diagonal form by an orthogonal similiarity transformation[6]

$$I = \mathcal{O} I_D \mathcal{O}^{-1}, \quad I_D = \begin{pmatrix} I_1 & 0 & 0 \\ 0 & I_2 & 0 \\ 0 & 0 & I_3 \end{pmatrix} \tag{4.24}$$

An orthogonal matrix $\mathcal{O}$ is either a rotation or a rotation times P, and the P's can be commuted through I_D without changing its form, so there is a rotation $\mathcal{R}$ which brings the inertia tensor into diagonal form. The axes of this new coordinate system are known as the **principal axes**.

Tire balancing

Consider a rigid body rotating on an axle, and therefore about a fixed axis. What total force and torque will the axle exert? First, $\dot{\vec{R}} = \vec{\omega} \times \vec{R}$, so

$$\ddot{\vec{R}} = \dot{\vec{\omega}} \times \vec{R} + \vec{\omega} \times \dot{\vec{R}} = \dot{\vec{\omega}} \times \vec{R} + \vec{\omega} \times (\omega \times \vec{R}) = \dot{\vec{\omega}} \times \vec{R} + \vec{\omega}(\vec{\omega} \cdot \vec{R}) + \vec{R}\omega^2.$$

If the axis is fixed, $\vec{\omega}$ and $\dot{\vec{\omega}}$ are in the same direction, so the first term is perpendicular to the other two. If we want the total force to be zero[7], $\ddot{\vec{R}} = 0$, so

$$\vec{R} \cdot \ddot{\vec{R}} = 0 = 0 + (\vec{\omega} \cdot \vec{R})^2 - R^2\omega^2.$$

Thus the angle between $\vec{\omega}$ and $\vec{R}$ is 0 or π, and the center of mass must lie on the axis of rotation. This is the condition of static balance if the axis of rotation is horizontal in a gravitational field. Consider a car

[6] This should be proven in any linear algebra course. For example, see [1], Theorem 6 in Section 6.3.

[7] Here we are ignoring any constant force compensating the force exerted by the road which is holding the car up!

tire: to be stable at rest at any angle, $\vec{R}$ must lie on the axis or there will be a gravitational torque about the axis, causing rotation in the absense of friction. If the tire is not statically balanced, this force will rotate rapidly with the tire, leading to vibrations of the car.

Even if the net force is 0, there might be a torque. $\vec{\tau} = \dot{\vec{L}} = d(I \cdot \vec{\omega})/dt$. If $I \cdot \vec{\omega}$ is not parallel to $\vec{\omega}$ it will rotate with the wheel, and so $\dot{\vec{L}}$ will rapidly oscillate. This is also not good for your axle. If, however, $\vec{\omega}$ is parallel to one of the principal axes, $I \cdot \vec{\omega}$ is parallel to $\vec{\omega}$, so if $\vec{\omega}$ is constant, so is $\vec{L}$, and $\vec{\tau} = 0$. The process of placing small weights around the tire to cause one of the principal axes to be aligned with the axle is called **dynamical balancing**.

Every rigid body has its principal axes; the problem of finding them and the moments of inertia about them, given the inertia tensor I_{ij} in some coordiate system, is a mathematical question of finding a rotation $\mathcal{R}$ and "eigenvalues" I_1, I_2, I_3 (not components of a vector) such that equation 4.24 holds, with $\mathcal{R}$ in place of $\mathcal{O}$. The vector $\vec{v}_1 = \mathcal{R}\begin{pmatrix}1\\0\\0\end{pmatrix}$ is then an eigenvector, for

$$I \cdot \vec{v}_1 = \mathcal{R} I_D \mathcal{R}^{-1} \mathcal{R} \begin{pmatrix}1\\0\\0\end{pmatrix} = \mathcal{R} I_D \begin{pmatrix}1\\0\\0\end{pmatrix} = I_1 \mathcal{R} \begin{pmatrix}1\\0\\0\end{pmatrix} = I_1 \vec{v}_1.$$

Similarly $I \cdot \vec{v}_2 = I_2 \vec{v}_2$ and $I \cdot \vec{v}_3 = I_3 \vec{v}_3$, where $\vec{v}_2$ and $\vec{v}_3$ are defined the same way, starting with $\hat{e}_2$ and $\hat{e}_3$ instead of $\hat{e}_1$. Note that, in general, I acts simply as a multiplier only for multiples of these three vectors individually, and not for sums of them. On a more general vector I will change the direction as well as the length.

Note that the I_i are all ≥ 0, for given any vector $\vec{n}$,

$$\vec{n} \cdot I \cdot \vec{n} = \sum_\alpha m_\alpha [r_\alpha^2 n^2 - (\vec{r}_\alpha \cdot \vec{n})^2] = \sum_\alpha m_\alpha r_\alpha^2 n^2 (1 - \cos^2 \theta_\alpha) \geq 0,$$

so all the eigenvalues must be ≥ 0. It will be equal to zero only if all massive points of the body are in the $\pm\vec{n}$ directions, in which case the rigid body must be a thin line.

Finding the eigenvalues I_i is easier than finding the rotation $\mathcal{R}$. Consider the matrix $I - \lambda \mathbb{1}$, which has the same eigenvectors as I,

but with eigenvalues $I_i - \lambda$. Then if λ is one of the eigenvalues of I_i, this matrix will annihilate $\vec{v}_i$, so $I_i - \lambda$ is a singular matrix with zero determinant. Thus the equation $\det(I - \lambda \mathbb{1}) = 0$, which is a cubic equation in λ, gives as its roots the eigenvalues of I.

4.4 Dynamics

4.4.1 Euler's Equations

So far, we have been working in an inertial coordinate system $\mathcal{O}$. In complicated situations this is rather unnatural; it is more natural to use a coordiate system $\mathcal{O}'$ fixed in the rigid body. In such a coordinate system, the vector one gets by differentiating the coefficients of a vector $\vec{b} = \sum b'_i \hat{e}'_i$ differs from the inertial derivative $\dot{\vec{b}}$ as given in Eq. 4.7. For the time derivative of the angular momentum, we have

$$\begin{aligned} \vec{\tau} = \frac{d\vec{L}}{dt} &= \left(\frac{d\vec{L}}{dt}\right)_b + \vec{\omega} \times \vec{L} \\ &= \sum_{ij} \frac{d(I'_{ij}\omega'_j)}{dt}\hat{e}'_i + \vec{\omega} \times (I' \cdot \vec{\omega}), \end{aligned}$$

where we have either a system rotating about a fixed point $\widetilde{R}$, with $\vec{\tau}$, $\vec{L}$, and I'_{ij} all evaluated about that fixed point, or we are working about the center of mass, with $\vec{\tau}$, $\vec{L}$, and I'_{ij} all evaluated about the center of mass, even if it is in motion. Now in the $\mathcal{O}'$ frame, all the masses are at fixed positions, so I'_{ij} is constant, and the first term is simply $I \cdot (d\omega/dt)_b$, which by (4.8) is simply $\dot{\vec{\omega}}$. Thus we have (in the body coordinate system)

$$\vec{\tau} = I' \cdot \dot{\vec{\omega}} + \vec{\omega} \times (I' \cdot \omega). \tag{4.25}$$

We showed that there is always a choice of cartesian coordinates mounted on the body along the principal axes. For the rest of this section we will use this body-fixed coordinate system, so we will drop the primes.

The torque not only determines the rate of change of the angular momentum, but also does work in the system. For a system rotating

about a fixed point, we see from the expression (4.13), $T = \frac{1}{2}\vec{\omega} \cdot I \cdot \vec{\omega}$, that

$$\frac{dT}{dt} = \frac{1}{2}\dot{\vec{\omega}} \cdot I \cdot \vec{\omega} + \frac{1}{2}\vec{\omega} \cdot \dot{I} \cdot \vec{\omega} + \frac{1}{2}\vec{\omega} \cdot I \cdot \dot{\vec{\omega}}.$$

The first and last terms are equal because the inertia tensor is symmetric, $I_{ij} = I_{ji}$, and the middle term vanishes in the body-fixed coordinate system because all particle positions are fixed. Thus $dT/dt = \vec{\omega} \cdot I \cdot \dot{\vec{\omega}} = \vec{\omega} \cdot \dot{\vec{L}} = \vec{\omega} \cdot \vec{\tau}$. Thus the kinetic energy changes due to the work done by the external torque. Therefore, of course, if there is no torque the kinetic energy is constant.

We will write out explicitly the components of Eq. 4.25. In evaluating τ_1, we need the first component of the second term,

$$[(\omega_1, \omega_2, \omega_3) \times (I_1\omega_1, I_2\omega_2, I_3\omega_3)]_1 = (I_3 - I_2)\omega_2\omega_3.$$

Inserting this and the similar expressions for the other components into Eq. (4.25), we get **Euler's equations**

$$\begin{aligned} \tau_1 &= I_1\dot{\omega}_1 + (I_3 - I_2)\omega_2\omega_3, \\ \tau_2 &= I_2\dot{\omega}_2 + (I_1 - I_3)\omega_1\omega_3, \\ \tau_3 &= I_3\dot{\omega}_3 + (I_2 - I_1)\omega_1\omega_2. \end{aligned} \tag{4.26}$$

Using these equations we can address several situations of increasing difficulty.

First, let us ask under what circumstances the angular velocity will be fixed in the absense of a torque. As $\vec{\tau} = \dot{\vec{\omega}} = 0$, from the 1-component equation we conclude that $(I_2 - I_3)\omega_2\omega_3 = 0$. Then either the moments are equal ($I_2 = I_3$) or one of the two components ω_2 or ω_3 must vanish. Similarly, if $I_1 \neq I_2$, either ω_1 or ω_2 vanishes. So the only way more than one component of $\vec{\omega}$ can be nonzero is if two or more of the principal moments are equal. In this case, the principal axes are not uniquely determined. For example, if $I_1 = I_2 \neq I_3$, the third axes is unambiguously required as one of the principle axes, but any direction in the (12)-plane will serve as the second principal axis. In this case we see that $\vec{\tau} = \dot{\vec{\omega}} = 0$ implies either $\vec{\omega}$ is along the z-axis ($\omega_1 = \omega_2 = 0$) or it lies in the (12)-plane, ($\omega_3 = 0$). In any case, the angular velocity is

constant in the absence of torques only if it lies along a principal axis of the body.

As our next example, consider an axially symmetric body with no external forces or torques acting on it. Then $\dot{\vec{R}}$ is a constant, and we will choose to work in an inertial frame where $\vec{R}$ is fixed at the origin. Choosing our body-fixed coordinates with z along the axis of symmetry, our axes are principal ones and $I_1 = I_2$, so we have

$$\begin{aligned} I_1\dot{\omega}_1 &= (I_1 - I_3)\omega_2\omega_3, \\ I_1\dot{\omega}_2 &= (I_3 - I_1)\omega_1\omega_3, \\ I_3\dot{\omega}_3 &= (I_1 - I_2)\omega_1\omega_2 = 0. \end{aligned}$$

We see that ω_3 is a constant. Let $\Omega = \omega_3(I_3 - I_1)/I_1$. Then we see that

$$\dot{\omega}_1 = -\Omega\omega_2, \qquad \dot{\omega}_2 = \Omega\omega_1.$$

Differentiating the first and plugging into the second, we find

$$\ddot{\omega}_1 = -\Omega\dot{\omega}_2 = -\Omega^2\omega_1,$$

which is just the harmonic oscillator equation. So $\omega_1 = A\cos(\Omega t + \phi)$ with some arbitrary amplitude A and constant phase ϕ, and $\omega_2 = -\dot{\omega}_1/\Omega = A\sin(\Omega t + \phi)$. We see that, in the body-fixed frame, the angular velocity rotates about the axis of symmetry in a circle, with arbitrary radius A, and a period $2\pi/\Omega$. The angular velocity vector $\vec{\omega}$ is therefore sweeping out a cone, called the **body cone** of precession with a half-angle $\phi_b = \tan^{-1} A/\omega_3$. Note the length of $\vec{\omega}$ is fixed.

What is happening in the lab frame? The kinetic energy $\frac{1}{2}\vec{\omega}\cdot\vec{L}$ is constant, as is the vector $\vec{L}$ itself. As the length of a vector is frame independent, $|\vec{\omega}|$ is fixed as well. Therefore the angle between them, called the **lab angle**, is constant,

$$\cos\phi_L = \frac{\vec{\omega}\cdot\vec{L}}{|\vec{\omega}||\vec{L}|} = \frac{2T}{|\vec{\omega}||\vec{L}|} = \text{constant}.$$

Thus $\vec{\omega}$ rotates about $\vec{L}$ in a cone, called the laboratory cone.

Note that ϕ_b is the angle between $\vec{\omega}$ and the z-axis of the body, while ϕ_L is the angle between $\vec{\omega}$ and $\vec{L}$, so they are not the same angle in two different coordinate systems.

The situation is a bit hard to picture. In the body frame it is hard to visualize $\vec{\omega}$, although that is the negative of the angular velocity of the universe in that system. In the lab frame the body is instantanously rotating about the axis $\vec{\omega}$, but this axis is not fixed in the body. At any instant, the points on this line are not moving, and we may think of the body rolling without slipping on the lab cone, with $\vec{\omega}$ the momentary line of contact. Thus the body cone rolls on the lab cone without slipping.

The Poinsot construction

This idea has an extension to the more general case where the body has no symmetry. The motion in this case can be quite complex, both for analytic solution, because Euler's equations are nonlinear, and to visualize, because the body is rotating and bobbing around in a complicated fashion. But as we are assuming there are no external forces or torques, the kinetic energy and total angular momentum vectors are constant, and this will help us understand the motion. To do so we construct an abstract object called the inertia ellipsoid. Working in the body frame, consider that the equation

$$2T = \sum_{ij} \omega_i I_{ij} \omega_j = f(\vec{\omega})$$

is a quadratic equation for $\vec{\omega}$, with constant coefficients, which therefore determines an ellipsoid[8] in the space of possible values of $\vec{\omega}$. This is called the **inertia ellipsoid**[9]. It is fixed in the body, and so if we were to scale it by some constant to change units from angular velocity to position, we could think of it as a fixed ellipsoid in the body itself, centered at the center of mass. At every moment the instantanous value of $\vec{\omega}$ must lie on this ellipsoid, so $\vec{\omega}(t)$ sweeps out a path on this ellipsoid called the **polhode**.

[8] We assume the body is not a thin line, so that I is a positive definite matrix (all its eigenvalues are strictly > 0), so the surface defined by this equation is bounded.

[9] Exactly which quantity forms the inertia ellipsoid varies by author. Goldstein scales $\vec{\omega}$ by a constant $1/\sqrt{2T}$ to form an object ρ whose ellipsoid he calls the inertia ellipsoid. Landau and Lifshitz discuss an ellipsoid of $\vec{L}$ values but don't give it a name. They then call the corresponding path swept out by $\vec{\omega}$ the polhode, as we do.

If we go to the lab frame, we see this ellipsoid fixed in and moving with the body. The instantaneous value of $\vec{\omega}$ still lies on it. In addition, the component of $\vec{\omega}$ in the (fixed) $\vec{L}$ direction is fixed, and as the center of mass is fixed, the point corresponding to $\vec{\omega}$ lies in a plane perpendicular to $\vec{L}$ a fixed distance from the center of mass, known as the **invariant plane**. Finally we note that the normal to the surface of the ellipsoid $f(\vec{\omega}) = 2T$ is parallel to $\nabla f = 2I \cdot \vec{\omega} = 2\vec{L}$, so the ellipsoid of inertia is tangent to the invariant plane at the point $\vec{\omega}(t)$. The path that $\vec{\omega}(t)$ sweeps out on the invariant plane is called the **herpolhode**. At this particular moment, the point corresponding to $\vec{\omega}$ in the body is not moving, so the inertia ellipsoid is rolling, not slipping, on the invariant plane.

In general, if there is no special symmetry, the inertia ellipsoid will not be axially symmetric, so that in order to roll on the fixed plane and keep its center at a fixed point, it will need to bob up and down. But in the special case with axial symmetry, the inertia ellipsoid will also have this symmetry, so it can roll about a circle, with its symmetry axis at a fixed angle relative to the invariant plane. In the body frame, ω_3 is fixed and the polhode moves on a circle of radius $A = \omega \sin\phi_b$. In the lab frame, $\vec{\omega}$ rotates about $\vec{L}$, so it sweeps out a circle of radius $\omega \sin\phi_L$ in the invariant plane. One circle is rolling on the other, and the polhode rotates about its circle at the rate Ω in the body frame, so the angular rate at which the herpolhode rotates about $\vec{L}$, Ω_L, is

$$\Omega_L = \Omega \frac{\text{circumference of polhode circle}}{\text{circumference of herpolhode circle}} = \frac{I_3 - I_1}{I_1}\omega_3 \frac{\sin\phi_b}{\sin\phi_L}.$$

Stability of rotation about an axis

We have seen that the motion of a isolated rigid body is simple only if the angular velocity is along one of the principal axes, and can be very complex otherwise. However, it is worth considering what happens if $\vec{\omega}$ is very nearly, but not exactly, along one of the principal axes, say z. Then we may write $\vec{\omega} = \omega_3\hat{e}_3 + \vec{\epsilon}$ in the body coordinates, and assume $\epsilon_3 = 0$ and the other components are small. We treat Euler's equations to first order in the small quantity $\vec{\epsilon}$. To this order, $\dot{\omega}_3 = (I_1 - I_2)\epsilon_1\epsilon_2/I_3 \approx 0$, so ω_3 may be considered a constant. The

other two equations give

$$\begin{aligned} \dot{\omega}_1 = \dot{\epsilon}_1 &= \frac{I_2 - I_3}{I_1}\epsilon_2\omega_3 \\ \dot{\omega}_2 = \dot{\epsilon}_2 &= \frac{I_3 - I_1}{I_2}\epsilon_1\omega_3 \end{aligned}$$

so

$$\ddot{\epsilon}_1 = \frac{I_2 - I_3}{I_1}\frac{I_3 - I_1}{I_2}\omega_3^2\epsilon_1.$$

What happens to $\vec{\epsilon}(t)$ depends on the sign of the coefficient, or the sign of $(I_2 - I_3)(I_3 - I_1)$. If it is negative, ϵ_1 oscillates, and indeed $\vec{\epsilon}$ rotates about z just as we found for the symmetric top. This will be the case if I_3 is either the largest or the smallest eigenvalue. If, however, it is the middle eigenvalue, the constant will be positive, and the equation is solved by exponentials, one damping out and one growing. Unless the initial conditions are perfectly fixed, the growing piece will have a nonzero coefficient and $\vec{\epsilon}$ will blow up. Thus a rotation about the intermediate principal axis is unstable, while motion about the axes with the largest and smallest moments are stable. For the case where two of the moments are equal, the motion will be stable about the third, and slightly unstable ($\vec{\epsilon}$ will grow linearly instead of exponentially with time) about the others.

An interesting way of understanding this stability or instability of rotation close to a principle axes involves another ellipsoid we can define for the free rigid body, an ellipsoid of possible angular momentum values. Of course in the inertial coordinates $\vec{L}$ is constant, but in body fixed language the coordinates vary with time, though the length of $\vec{L}$ is still constant. In addition, the conservation of kinetic energy

$$2T = \vec{L} \cdot I^{-1} \cdot \vec{L}$$

(where I^{-1} is the inverse of the moment of inertia matrix) gives a quadratic equation for the three components of $\vec{L}$, just as we had for $\vec{\omega}$ and the ellipsoid of inertia. The path of $\vec{L}(t)$ on this ellipsoid is on the intersection of the ellisoid with a sphere of radius $|\vec{L}|$, for the length is fixed.

If $\vec{\omega}$ is near the principle axis with the largest moment of inertia, $\vec{L}$ lies near the major axis of the ellipsoid. The sphere is nearly circumscribing the ellipsoid, so the intersection consists only of two small loops surrounding each end of the major axis. Similiarly if $\vec{\omega}$ is near the smallest moment, the sphere is nearly inscribed by the ellipsoid, and again the possible values of $\vec{L}$ lie close to either end of the minor axis. Thus the subsequent motion is confined to one of these small loops. But if $\vec{\omega}$ starts near the intermediate principle axis, $\vec{L}$ does likewise, and the intersection consists of two loops which extend from near one end to near the other of the intermediate axis, and the possible continuous motion of $\vec{L}$ is not confined to a small region of the ellipsoid.

Because the rotation of the Earth flattens the poles, the Earth is approximately an **oblate** ellipsoid, with I_3 greater than $I_1 = I_2$ by about one part in 300. As ω_3 is 2π per siderial day, if $\vec{\omega}$ is not perfectly aligned with the axis, it will precess about the symmetry axis once every 10 months. This **Chandler wobble** is not of much significance, however, because the body angle $\phi_b \approx 10^{-6}$.

4.4.2 Euler angles

Up to this point we have managed to describe the motion of a rigid body without specifying its coordinates. This is not possible for most problems with external forces, for which the torque will generally depend on the orientation of the body. It is time to face up to the problem of using three generalized coordinates to describe the orientation.

In section 4.1.1 we described the orientation of a rigid body in terms of a rotation through a finite angle in a given direction, specified by ω. This does not give a simple parameterization of the matrix A, and it is more common to use an alternate description known as Euler angles. Here we describe the rotation A as a composition of three simpler rotations about specified coordinates, so that we are making a sequence of changes of coordinates

$$(x, y, z) \xrightarrow{R_z(\phi)} (x_1, y_1, z_1) \xrightarrow{R_{y_1}(\theta)} (x_2, y_2, z_2) \xrightarrow{R_{z_2}(\psi)} (x', y', z').$$

We have chosen three specific directions about which to make the three rotations, namely the original z-axis, the next y-axis, y_1, and then the

new z-axis, which is both z_2 and z'. This choice is not universal, but is the one generally used in quantum mechanics. Many of the standard classical mechanics texts[10] take the second rotation to be about the x_1-axis instead of y_1, but quantum mechanics texts[11] avoid this because the action of R_y on a spinor is real, while the action of R_x is not. While this does not concern us here, we prefer to be compatible with quantum mechanics discussions.

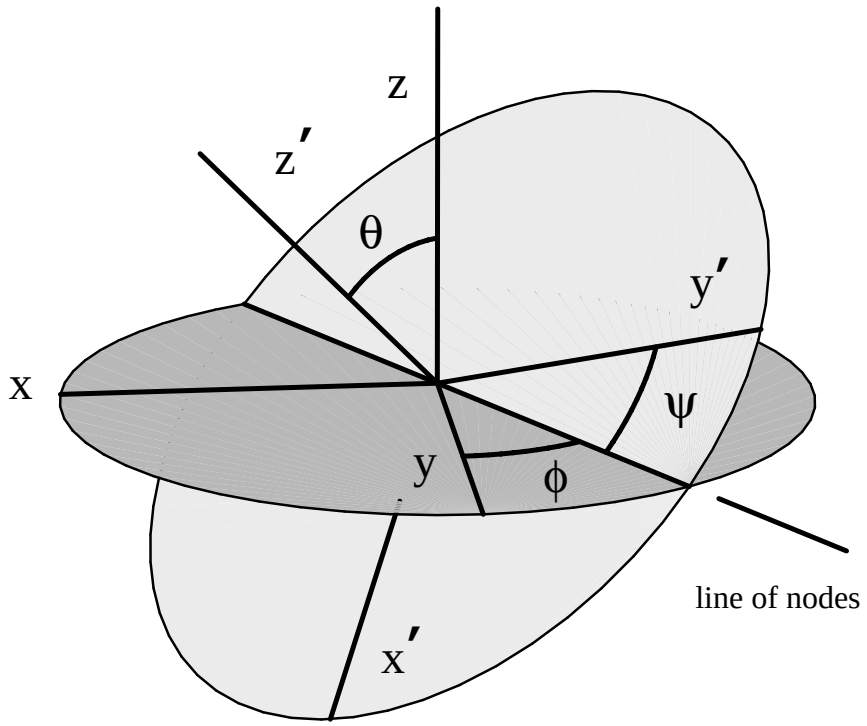


Figure 4.2: The Euler angles as rotations through ϕ, θ, ψ, about the z, y_1, and z_2 axes sequentially

This procedure is pictured in Figure 4.2. To see that any rotation can be written in this form, and to determine the range of the angles, we first discuss what fixes the y_1 axis. Notice that the rotation about the z-axis leaves z uneffected, so $z_1 = z$, Similiarly, the last rotation leaves

[10] See [2], [4], [6], [7], [8] and [12].
[11] For example [9] and [13].

the z_2 axis unchanged, so it is also the z' axis. The planes orthogonal to these axes are also left invariant[12]. These planes, the xy-plane and the $x'y'$-plane respectively, intersect in a line called the **line of nodes**[13]. These planes are also the x_1y_1 and x_2y_2 planes respectively, and as the second rotation $R_{y_1}(\theta)$ must map the first into the second plane, we see that y_1, which is unaffected by R_{y_1}, must be along the line of nodes. We choose between the two possible orientations of y_1 to keep the necessary θ angle in $[0, \pi]$. The angles ϕ and ψ are then chosen $\in [0, 2\pi)$ as necessary to map $y \to y_1$ and $y_1 \to y'$ respectively.

While the rotation about the z-axis leaves z uneffected, it rotates the x and y components by the matrix (4.4). Thus in three dimensions, a rotation about the z axis is represented by

$$R_z(\phi) = \begin{pmatrix} \cos\phi & \sin\phi & 0 \\ -\sin\phi & \cos\phi & 0 \\ 0 & 0 & 1 \end{pmatrix}. \tag{4.27}$$

Similarly a rotation through an angle θ about the current y axis has a similar form

$$R_y(\theta) = \begin{pmatrix} \cos\theta & 0 & -\sin\theta \\ 0 & 1 & 0 \\ \sin\theta & 0 & \cos\theta \end{pmatrix}. \tag{4.28}$$

The reader needs to assure himself, by thinking of the rotations as active transformations, that the action of the matrix R_y after having applied R_z produces a rotation about the y_1-axis, not the original y-axis.

The full rotation $A = R_z(\psi) \cdot R_y(\theta) \cdot R_z(\phi)$ can then be found simply by matrix multiplication:

$$\begin{aligned} A(\phi, \theta, \psi) &= \\ &\begin{pmatrix} \cos\psi & \sin\psi & 0 \\ -\sin\psi & \cos\psi & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \cos\theta & 0 & -\sin\theta \\ 0 & 1 & 0 \\ \sin\theta & 0 & \cos\theta \end{pmatrix} \begin{pmatrix} \cos\phi & \sin\phi & 0 \\ -\sin\phi & \cos\phi & 0 \\ 0 & 0 & 1 \end{pmatrix} \\ &= \end{aligned} \tag{4.29}$$

[12] although the points in the planes are rotated by 4.4.

[13] The case where the xy and $x'y'$ are identical, rather than intersecting in a line, is exceptional, corresponding to $\theta = 0$ or $\theta = \pi$. Then the two rotations about the z-axis add or subtract, and many choices for the Euler angles (ϕ, ψ) will give the same full rotation.

$$\begin{pmatrix} -\sin\phi\sin\psi+\cos\theta\cos\phi\cos\psi & \cos\phi\sin\psi+\cos\theta\sin\phi\cos\psi & -\sin\theta\cos\psi \\ -\sin\phi\cos\psi-\cos\theta\cos\phi\sin\psi & \cos\phi\cos\psi-\cos\theta\sin\phi\sin\psi & \sin\theta\sin\psi \\ \sin\theta\cos\phi & \sin\theta\sin\phi & \cos\theta \end{pmatrix}.$$

We need to reexpress the kinetic energy in terms of the Euler angles and their time derivatives. From the discussion of section 4.2, we have

$$\Omega' = -A(t)\cdot\frac{d}{dt}A^{-1}(t)$$

The inverse matrix is simply the transpose, so finding Ω' can be done by straightforward differentiation and matrix multiplication[14]. The result is

$$\Omega' = \tag{4.30}$$
$$\begin{pmatrix} 0 & \dot\psi+\dot\phi\cos\theta & -\dot\theta\cos\psi-\dot\phi\sin\theta\sin\psi \\ -\dot\psi-\dot\phi\cos\theta & 0 & \dot\theta\sin\psi-\dot\phi\sin\theta\cos\psi \\ \dot\theta\cos\psi+\dot\phi\sin\theta\sin\psi & -\dot\theta\sin\psi+\dot\phi\sin\theta\cos\psi & 0 \end{pmatrix}.$$

Note Ω' is antisymmetric as expected, so it can be recast into the axial vector ω

$$\begin{aligned} \omega_1' &= \Omega_{23}' = \dot\theta\sin\psi-\dot\phi\sin\theta\cos\psi, \\ \omega_2' &= \Omega_{31}' = \dot\theta\cos\psi+\dot\phi\sin\theta\sin\psi, \\ \omega_3' &= \Omega_{12}' = \dot\psi+\dot\phi\cos\theta. \end{aligned} \tag{4.31}$$

This expression for $\vec\omega$ gives the necessary velocities for the kinetic energy term (4.19 or 4.21) in the Lagrangian, which becomes

$$L = \frac{1}{2}M\tilde V^2 + M\tilde V\cdot\left(\vec\omega\times\vec B\right)+\frac{1}{2}\vec\omega\cdot I^{(\tilde R)}\cdot\vec\omega - U(\tilde R,\theta,\psi,\phi), \tag{4.32}$$

or

$$L = \frac{1}{2}M\vec V^{\,2} + \frac{1}{2}\vec\omega\cdot I^{(cm)}\cdot\vec\omega - -U(\vec R,\theta,\psi,\phi), \tag{4.33}$$

with $\vec\omega=\sum_i\omega_i'\hat e_i'$ given by (4.31).

[14]Verifying the above expression for A and the following one for Ω' is a good application for a student having access to a good symbolic algebra computer program. Both Mathematica and Maple handle the problem nicely.

4.4.3 The symmetric top

Now let us consider an example with external forces which constrain one point of a symmetrical top to be stationary. Then we choose this to be the fixed point, at the origin $\tilde{R} = 0$, and we choose the body-fixed z'-axis to be along the axis of symmetry. Of course the center of mass in on this axis, so $\vec{R} = (0, 0, \ell)$ in body-fixed coordinates. We will set up the motion by writing the Lagrangian from the forms for the kinetic and potential energy, due entirely to the gravitational field[15].

$$\begin{aligned} T &= \frac{1}{2}(\omega_1^2 + \omega_2^2)I_1 + \frac{1}{2}\omega_3^2 I_3 \\ &= \frac{1}{2}\left(\dot{\phi}^2 \sin^2\theta + \dot{\theta}^2\right) I_1 + \frac{1}{2}\left(\dot{\phi}\cos\theta + \dot{\psi}\right)^2 I_3, \qquad (4.34) \\ U &= Mgz_{\rm cm} = Mg\ell\left(A^{-1}\right)_{zz} = Mg\ell\cos\theta. \qquad (4.35) \end{aligned}$$

So $L = T - U$ is independent of ϕ, ψ, and the corresponding momenta

$$\begin{aligned} p_\phi &= \dot{\phi}\sin^2\theta I_1 + \left(\dot{\phi}\cos\theta + \dot{\psi}\right)\cos\theta I_3 \\ &= \dot{\phi}\sin^2\theta I_1 + \cos\theta\omega_3 I_3, \\ p_\psi &= \left(\dot{\phi}\cos\theta + \dot{\psi}\right) I_3 = \omega_3 I_3 \end{aligned}$$

are constants of the motion. Let us use parameters $a = p_\psi/I_1$ and $b = p_\phi/I_1$, which are more convenient, to parameterize the motion, instead of p_ϕ, p_ψ, or even ω_3, which is also a constant of the motion and might seem physically a more natural choice. A third constant of the motion is the energy,

$$E = T + U = \frac{1}{2}I_1\left(\dot{\theta}^2 + \dot{\phi}^2\sin^2\theta\right) + \frac{1}{2}\omega_3^2 I_3 + Mg\ell\cos\theta.$$

Solving for $\dot{\phi}$ from $p_\phi = I_1 b = \dot{\phi}\sin^2\theta I_1 + I_1 a\cos\theta$,

$$\begin{aligned} \dot{\phi} &= \frac{b - a\cos\theta}{\sin^2\theta}, \qquad (4.36) \\ \dot{\psi} &= \omega_3 - \dot{\phi}\cos\theta = \frac{I_1 a}{I_3} - \frac{b - a\cos\theta}{\sin^2\theta}\cos\theta, \qquad (4.37) \end{aligned}$$

[15] As we did in discussing Euler's equations, we drop the primes on ω_i and on I_{ij} even though we are evaluating these components in the body fixed coordinate system. The coordinate z, however, is still a lab coordinate, with $\hat{e}_z$ pointing upward.

Then E becomes

$$E = \frac{1}{2} I_1 \dot{\theta}^2 + U'(\theta) + \frac{1}{2} I_3 \omega_3^2,$$

where

$$U'(\theta) := \frac{1}{2} I_1 \frac{(b - a\cos\theta)^2}{\sin^2\theta} + Mg\ell\cos\theta.$$

The term $\frac{1}{2} I_3 \omega_3^2$ is an ignorable constant, so we consider $E' := E - \frac{1}{2} I_3 \omega_3^2$ as the third constant of the motion, and we now have a one dimensional problem for $\theta(t)$, with a first integral of the motion. Once we solve for $\theta(t)$, we can plug back in to find $\dot{\phi}$ and $\dot{\psi}$.

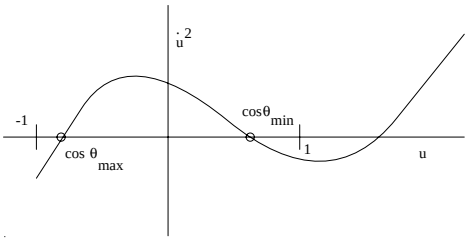
Substitute $u = \cos\theta$, $\dot{u} = -\sin\theta\dot{\theta}$, so

$$E' = \frac{I_1 \dot{u}^2}{2(1-u^2)} + \frac{1}{2} I_1 \frac{(b-au)^2}{1-u^2} + Mg\ell u,$$

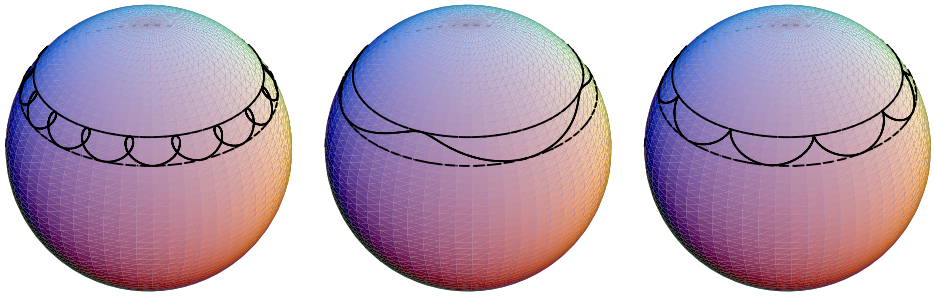
or

$$\dot{u}^2 = (1-u^2)(\alpha - \beta u) - (b - au)^2 =: f(u), \tag{4.38}$$

with $\alpha = 2E'/I_1$, $\beta = 2Mg\ell/I_1$. $f(u)$ is a cubic with a positive u^3 term, and is negative at $u = \pm 1$, where the first term vanishes, and which are also the limits of the physical range of values of u. If there are to be any allowed values for $\dot{u}^2$, $f(u)$ must be nonnegative somewhere in $u \in [-1, 1]$, so f must look very much like what is shown.



To visualize what is happening, note that a point on the symmetry axis moves on a sphere, with θ and ϕ representing the usual spherical coordinates, as can be seen by examining what A^{-1} does to $(0, 0, z')$. So as θ moves back and forth between $\theta_{\min}$ and $\theta_{\max}$, the top is wobbling closer and further from the vertical, called **nutation**. At the same time, the symmetry axis is **precessing**, rotating about the vertical



$\theta' = 52°$ $\theta' = 44°$ $\theta' = \theta_{\min}$

Figure 4.3: Possible loci for a point on the symmetry axis of the top. The axis nutates between $\theta_{\min} = 50°$ and $\theta_{\max} = 60°$

axis, at a rate $\dot{\phi}$ which is not constant but a function of θ (Eq. 4.36). Qualitatively we may distinguish three kinds of motion, depending on the values of $\dot{\phi}$ at the turning points in θ. These in turn depend on the initial conditions and the parameters of the top, expressed in a, b, and $\theta_{\min}$, $\theta_{\max}$. If the value of $u' = \cos\theta'$ at which $\dot{\phi}$ vanishes is within the range of nutation, then the precession will be in different directions at $\theta_{\min}$ and $\theta_{\max}$, and the motion is as in Fig. 4.3a. On the other hand, if $\theta' = \cos^{-1}(b/a) \notin [\theta_{\min}, \theta_{\max}]$, the precession will always be in the same direction, although it will speed up and slow down. We then get a motion as in Fig. 4.3b. Finally, it is possible that $\cos\theta_{\min} = b/a$, so that the precession stops at the top, as in Fig. 4.3c. This special case is of interest, because if the top's axis is held still at an angle to the vertical, and then released, this is the motion we will get.

Exercises

4.1 Prove the following properties of matrix algebra:
(a) Matrix multiplication is associative: $A \cdot (B \cdot C) = (A \cdot B) \cdot C$.
(b) $(A \cdot B)^T = B^T \cdot A^T$, where A^T is the **transpose** of A, that is $(A^T)_{ij} := A_{ji}$.
(c) If A^{-1} and B^{-1} exist, $(A \cdot B)^{-1} = B^{-1} \cdot A^{-1}$.
(d) The complex conjugate of a matrix $(A^*)_{ij} = A^*_{ij}$ is the matrix with every element complex conjugated. The **hermitean conjugate** $A^\dagger$ is the

transpose of that, $A^\dagger := (A^*)^T = (A^T)^*$, with $(A^\dagger)_{ij} := A^*_{ji}$. Show that $(A \cdot B)^* = A^* \cdot B^*$ and $(A \cdot B)^\dagger = B^\dagger \cdot A^\dagger$.

4.2 In section (4.1) we considered reexpressing a vector $\vec{V} = \sum_i V_i \hat{e}_i$ in terms of new orthogonal basis vectors. If the new vectors are $\vec{e}\,'_i = \sum_j A_{ij}\hat{e}_j$, we can also write $\hat{e}_i = \sum_j A_{ji}\vec{e}\,'_j$, because $A^T = A^{-1}$ for an orthogonal transformation.
Consider now using a new basis $\vec{e}\,'_i$ which are *not* orthonormal. Then we must choose which of the two above expressions to generalize. Let $\hat{e}_i = \sum_j A_{ji}\vec{e}\,'_j$, and find the expressions for (a) $\vec{e}\,'_j$ in terms of $\hat{e}_i$; (b) V'_i in terms of V_j; and (c) V_i in terms of V'_j. Then show (d) that if a linear tranformation $\mathbf{T}$ which maps vectors $\vec{V} \to \vec{W}$ is given in the $\hat{e}_i$ basis by a matrix B_{ij}, in that $W_i = \sum B_{ij}V_j$, then the same transformation $\mathbf{T}$ in the $\vec{e}\,'_i$ basis is given by $C = A \cdot B \cdot A^{-1}$. This transformation of matrices, $B \to C = A \cdot B \cdot A^{-1}$, for an arbitrary invertible matrix A, is called a **similarity transformation**.

4.3 Two matrices B and C are called **similar** if there exists an invertible matrix A such that $C = A \cdot B \cdot A^{-1}$, and this transformation of B into C is called a similarity transformation, as in the last problem. Show that, if B and C are similar, (a) $\mathrm{Tr}\, B = \mathrm{Tr}\, C$; (b) $\det B = \det C$; (c) B and C have the same eigenvalues; (d) If A is orthogonal and B is symmetric (or antisymmetric), then C is symmetric (or antisymmetric).

4.4 From the fact that $AA^{-1} = 1$ for any invertible matrix, show that if $A(t)$ is a differentiable matrix-valued function of time,

$$\dot{A}\, A^{-1} = -A\frac{dA^{-1}}{dt}.$$

4.5 Show that a counterclockwise rotation through an angle θ about an axis in the direction of a unit vector $\hat{n}$ passing through the origin is given by the matrix

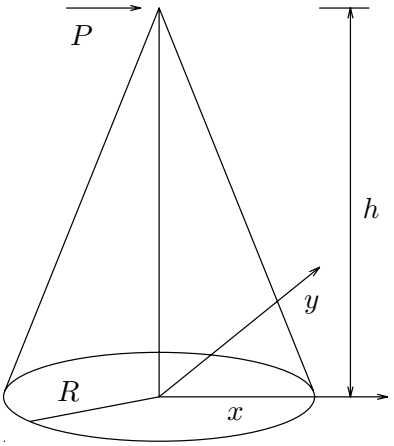
$$A_{ij} = \delta_{ij}\cos\theta + n_i n_j(1 - \cos\theta) - \epsilon_{ijk}n_k \sin\theta.$$

4.6 Consider a rigid body in the shape of a right circular cone of height h and a base which is a circle of radius R, made of matter with a uniform density ρ.

a) Find the position of the center of mass. Be sure to specify with respect to what.

b) Find the moment of inertia tensor in some suitable, well specified coordinate system about the center of mass.

c) Initially the cone is spinning about its symmetry axis, which is in the z direction, with angular velocity ω_0, and with no external forces or torques acting on it. At time $t = 0$ it is hit with a momentary laser pulse which imparts an impulse P in the x direction at the apex of the cone, as shown.

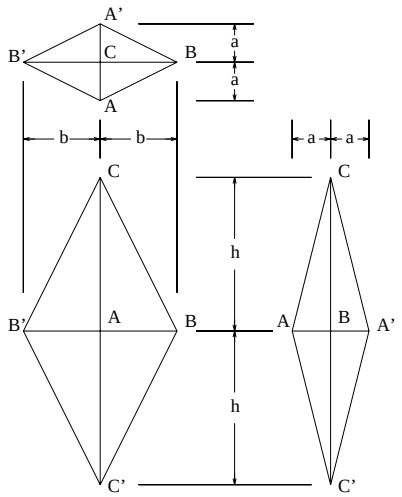


Describe the subsequent force-free motion, including, as a function of time, the angular velocity, angular momentum, and the position of the apex, in any inertial coordinate system you choose, provided you spell out the relation to the initial inertial coordinate system.

4.7 We defined the general rotation as $A = R_z(\psi) \cdot R_y(\theta) \cdot R_z(\phi)$. Work out the full expression for $A(\phi, \theta, \psi)$, and verify the last expression in (4.29). [For this and exercise 4.8, you might want to use a computer algebra program such as mathematica or maple, if one is available.]

4.8 Find the expression for $\vec{\omega}$ in terms of $\phi, \theta, \psi, \dot{\phi}, \dot{\theta}, \dot{\psi}$. [This can be done simply with computer algebra programs. If you want to do this by hand, you might find it easier to use the product form $A = R_3 R_2 R_1$, and the rather simpler expressions for $R\dot{R}^T$. You will still need to bring the result (for $R_1 \dot{R}_1^T$, for example) through the other rotations, which is somewhat messy.]

4.9 A diamond shaped object is shown in top, front, and side views. It is an octahedron, with 8 triangular flat faces.



It is made of solid aluminum of uniform density, with a total mass M. The dimensions, as shown, satisfy $h > b > a$.
(a) Find the moment of inertia tensor about the center of mass, clearly specifying the coordinate system chosen.
(b) About which lines can a stable spinning motion, with fixed $\vec{\omega}$, take place, assuming no external forces act on the body?

4.10 From the expression 4.38 for $u = \cos\theta$ for the motion of the symmetric top, we can derive a function for the time $t(u)$ as an indefinite integral

$$t(u) = \int^u f^{-1/2}(z)\, dz.$$

For values which are physically realizable, the function f has two (generically distinct) roots, $u_X \leq u_N$ in the interval $u \in [-1, 1]$, and one root $u_U \in [1, \infty)$, which does not correspond to a physical value of θ. The integrand is then generically an analytic function of z with square root branch points at u_N, u_X, u_U, and ∞, which we can represent on a cut Riemann sheet with cuts on the real axis, $[-\infty, u_X]$ and $[u_N, u_U]$, and $f(u) > 0$ for $u \in (u_X, u_N)$. Taking $t = 0$ at the time the top is at the bottom of a wobble, $\theta = \theta_{\max}, u = u_X$, we can find the time at which it first reaches another $u \in [u_X, u_N]$ by integrating along the real axis. But we could also use any other path in the upper half plane, as the integral of a complex function is independent of deformations of the path through regions where the function is analytic.
(a) Extend this definition to a function $t(u)$ defined for Im $u \geq 0$, with u not on a cut, and show that the image of this function is a rectangle in the complex t plane, and identify the pre-images of the sides. Call the width $T/2$ and the height $\tau/2$
(b) Extend this function to the lower half of the same Riemann sheet by allowing contour integrals passing through $[u_X, u_N]$, and show that this extends the image in t to the rectangle $(0, T/2) \times (-i\tau/2, i\tau/2)$.
(c) If the coutour passes through the cut $(-\infty, u_X]$ onto the second Riemann sheet, the integrand has the opposite sign from what it would have at the

corresponding point of the first sheet. Show that if the path takes this path onto the second sheet and reaches the point u, the value $t_1(u)$ thus obtained is $t_1(u) = -t_0(u)$, where $t_0(u)$ is the value obtained in (a) or (b) for the same u on the first Riemann sheet.
(d) Show that passing to the second Riemann sheet by going through the cut $[u_N, u_U]$ instead, produces a $t_2(u) = t_1 + T$.
(e) Show that evaluating the integral along two contours, Γ_1 and Γ_2, which differ only by Γ_1 circling the $[u_N, u_U]$ cut clockwise once more than Γ_2 does, gives $t_1 = t_2 + i\tau$.
(f) Show that any value of t can be reached by some path, by circling the $[u_N, u_U]$ as many times as necessary, and also by passing downwards through it and upwards through the $[-\infty, u_X]$ cut as often as necessary (perhaps reversed).
(g) Argue that thus means the function $u(t)$ is an analytic function from the complex t plane into the u complex plane, analytic except at the points $t = nT + i(m + \frac{1}{2})\tau$, where $u(t)$ has double poles. Note this function is doubly periodic, with $u(t) = u(t + nT + im\tau)$.
(g) Show that the function is then given by $u = \beta\,\wp(t - i\tau/2) + c$, where c is a constant, β is the constant from (4.38), and

$$\wp(z) = \frac{1}{z^2} + \sum_{\substack{m,n\in\mathbf{Z}\\(m,n)\neq 0}} \left(\frac{1}{(z - nT - mi\tau)^2} - \frac{1}{(nT + mi\tau)^2} \right)$$

is the Weierstrass' $\wp$-Function.
(h) Show that $\wp$ satisfies the differential equation

$$\wp'^2 = 4\wp^3 - g_2\wp - g_3,$$

where

$$g_2 = \sum_{\substack{m,n\in\mathbb{Z}\\(m,n)\neq(0,0)}} (mT + in\tau)^{-4}, \qquad g_3 = \sum_{\substack{m,n\in\mathbb{Z}\\(m,n)\neq(0,0)}} (mT + in\tau)^{-6}.$$

[Note that the Weierstrass function is defined more generally, using parameters $\omega_1 = T/2$, $\omega_2 = i\tau/2$, with the ω's permitted to be arbitrary complex numbers with differing phases.]

4.11 As a rotation about the origin maps the unit sphere into itself, one way to describe rotations is as a subset of maps $f : S^2 \to S^2$ of the (surface of the) unit sphere into itself. Those which correspond to rotations are clearly

one-to-one, continuous, and preserve the angle between any two paths which intersect at a point. This is called a conformal map. In addition, rotations preserve the distances between points. In this problem we show how to describe such mappings, and therefore give a representation for the rotations in three dimensions.

(a) Let N be the north pole $(0,0,1)$ of the unit sphere $\Sigma = \{(x,y,z), x^2 + y^2 + z^2 = 1\}$. Define the map from the rest of the sphere $s : \Sigma - \{N\} \to \mathbb{R}^2$ given by a stereographic projection, which maps each point on the unit sphere, other than the north pole, into the point (u,v) in the equatorial plane $(x,y,0)$ by giving the intersection with this plane of the straight line which joins the point $(x,y,z) \in \Sigma$ to the north pole. Find (u,v) as a function of (x,y,z), and show that the lengths of infinitesimal paths in the vicinity of a point are scaled by a factor $1/(1-z)$ independent of direction, and therefore that the map s preserves the angles between intersecting curves (*i.e.* is **conformal**).

(b) Show that the map $f((u,v)) \to (u',v')$ which results from first applying s^{-1}, then a rotation, and then s, is a conformal map from $\mathbb{R}^2$ into $\mathbb{R}^2$, except for the pre-image of the point which gets mapped into the north pole by the rotation.

By a general theorem of complex variables, any such map is analytic, so $f : u + iv \to u' + iv'$ is an analytic function except at the point $\xi_0 = u_0 + iv_0$ which is mapped to infinity, and ξ_0 is a simple pole of f. Show that $f(\xi) = (a\xi + b)/(\xi - \xi_0)$, for some complex a and b. This is the set of complex Mobius transformations, which are usually rewritten as

$$f(\xi) = \frac{\alpha\xi + \beta}{\gamma\xi + \delta},$$

where $\alpha, \beta, \gamma, \delta$ are complex constants. An overall complex scale change does not affect f, so the scale of these four complex constants is generally fixed by imposing a normalizing condition $\alpha\delta - \beta\gamma = 1$.

(c) Show that composition of Mobius transformations $f'' = f' \circ f : \xi \underset{f}{\longrightarrow} \xi' \underset{f'}{\longrightarrow} \xi''$ is given by matrix multiplication,

$$\begin{pmatrix} \alpha'' & \beta'' \\ \gamma'' & \delta'' \end{pmatrix} = \begin{pmatrix} \alpha' & \beta' \\ \gamma' & \delta' \end{pmatrix} \cdot \begin{pmatrix} \alpha & \beta \\ \gamma & \delta \end{pmatrix}.$$

(d) Not every mapping $s^{-1} \circ f \circ s$ is a rotation, for rotations need to preserve distances as well. We saw that an infinitesimal distance $d\ell$ on Σ is mapped by s to a distance $|d\xi| = d\ell/(1-z)$. Argue that the condition that $f : \xi \to \tilde{\xi}$

correspond to a rotation is that $d\tilde{\ell} \equiv (1-\tilde{z})|df/d\xi||d\xi| = d\ell$. Express this change of scale in terms of ξ and $\tilde{\xi}$ rather than z and $\tilde{z}$, and find the conditions on $\alpha, \beta, \gamma, \delta$ that insure this is true for all ξ. Together with the normalizing condition, show that this requires the matrix for f to be a unitary matrix with determinant 1, so that the set of rotations corresponds to the group $SU(2)$. The matrix elements are called Cayley-Klein parameters, and the real and imaginary parts of them are called the Euler parameters.

Chapter 5

Small Oscillations

5.1 Small oscillations about stable equilibrium

Consider a situation with N unconstrained generalized coordinates q_i described by a mass matrix M_{ij} and a potential $U(\{q_i\})$, and suppose that U has a local minimum at some point in configuration space, $q_i = q_{i0}$. Then this point is a stable equilibrium point, for the generalized force at that point is zero, and if the system is placed nearly at rest near that point, it will not have enough energy to move far away from that point. We may study the behavior of such motions by expanding the potential[1] in Taylor's series expansion in the deviations $\eta_i = q_i - q_{i0}$,

$$U(q_1, \ldots, q_N) = U(q_{i0}) + \sum_i \left.\frac{\partial U}{\partial q_i}\right|_0 \eta_i + \frac{1}{2}\sum_{ij} \left.\frac{\partial^2 U}{\partial q_i \partial q_j}\right|_0 \eta_i \eta_j + \ldots .$$

The constant $U(q_{i0})$ is of no interest, as only changes in potential matter, so we may as well set it to zero. In the second term, $-\left.\partial U/\partial q_i\right|_0$ is the generalized force at the equilibrium point, so it is zero. Thus the leading term in the expansion is the quadratic one, and we may approximate

$$U(\{q_i\}) = \frac{1}{2}\sum_{ij} A_{ij}\eta_i\eta_j, \quad \text{with} \quad A_{ij} = \left.\frac{\partial^2 U}{\partial q_i \partial q_j}\right|_0 . \tag{5.1}$$

[1] assumed to have continuous second derivatives.

Note that A is a constant symmetric real matrix.

The kinetic energy $T = \frac{1}{2}\sum M_{ij}\dot{\eta}_i\dot{\eta}_j$ is already second order in the small variations from equilibrium, so we may evaluate M_{ij}, which in general can depend on the coordinates q_i, at the equilibrium point, ignoring any higher order changes. Thus M_{ij} is a constant. Thus both the kinetic and potential energies are quadratic forms in the displacement η, which we think of as a vector in N-dimensional space. Thus we can write the energies in matrix form

$$T = \frac{1}{2}\dot{\eta}^T \cdot M \cdot \dot{\eta}, \qquad U = \frac{1}{2}\eta^T \cdot A \cdot \eta. \tag{5.2}$$

A and M are real symmetric matrices, and because any displacement corresponds to positive kinetic and nonnegative potential energies, they are positive (semi)definite matrices, meaning that all their eigenvalues are greater than zero, except that A may also have eigenvalues equal to zero (these are directions in which the stability is neutral to lowest order, but may be determined by higher order terms in the displacement).

Lagrange's equation of motion

$$0 = \frac{d}{dt}\frac{\partial L}{\partial \dot{\eta}_i} - \frac{\partial L}{\partial \eta_i} = \frac{d}{dt}M \cdot \dot{\eta} + A \cdot \eta = M \cdot \ddot{\eta} + A \cdot \eta \tag{5.3}$$

is not necessarily diagonal in the coordinate η. We shall use the fact that any real symmetric matrix can be diagonalized by a similarity transformation with an orthogonal matrix to reduce the problem to a set of independant harmonic oscillators. While both M and A can be diagonalized by an orthogonal transformation, they can not necessarily be diagonalized by the *same* one, so our procedure will be in steps:

1. Diagonalize M with an orthogonal transformation $\mathcal{O}_1$, transforming the coordinates to a new set $x = \mathcal{O}_1 \cdot \eta$.

2. Scale the x coordinates to reduce the mass matrix to the identity matrix. The new coordinates will be called y.

3. Diagonalize the new potential energy matrix with another orthogonal matrix $\mathcal{O}_2$, giving the final set of coordinates, $\xi = \mathcal{O}_2 \cdot y$. Note

this transformation leaves the kinetic energy matrix diagonal because the identity matrix is unaffected by similarity transformations.

The ξ are **normal modes**, modes of oscillation which are independent in the sense that they do not affect each other.

Let us do this in more detail. We are starting with the coordinates η and the real symmetric matrices A and M, and we want to solve the equations $M \cdot \ddot{\eta} + A \cdot \eta = 0$. In our first step, we use the matrix $\mathcal{O}_1$, which linear algebra guarantees exists, that makes $m = \mathcal{O}_1 \cdot M \cdot \mathcal{O}_1^{-1}$ diagonal. Note $\mathcal{O}_1$ is time-independent, so defining $x_i = \sum_j \mathcal{O}_{1\,ij}\eta_j$ also gives $\dot{x}_i = \sum_j \mathcal{O}_{1\,ij}\dot{\eta}_j$, and

$$\begin{aligned} T &= \frac{1}{2}\dot{\eta}^T \cdot M \cdot \dot{\eta} \\ &= \frac{1}{2}\dot{\eta}^T \cdot \left(\mathcal{O}_1^{-1} \cdot m \cdot \mathcal{O}_1\right) \cdot \dot{\eta} \\ &= \frac{1}{2}\left(\dot{\eta}^T \cdot \mathcal{O}_1^T\right) \cdot m \cdot (\mathcal{O}_1 \cdot \dot{\eta}) \\ &= \frac{1}{2}\left(\mathcal{O}_1 \cdot \dot{\eta}\right)^T \cdot m \cdot (\mathcal{O}_1 \cdot \dot{\eta}) \\ &= \frac{1}{2}\dot{x}^T \cdot m \cdot \dot{x}. \end{aligned}$$

Similarly the potential energy becomes $U = \frac{1}{2}x^T \cdot \mathcal{O}_1 \cdot A \cdot \mathcal{O}_1^{-1} \cdot x$. We know that the matrix m is diagonal, and the diagonal elements m_{ii} are all strictly positive. To begin the second step, define the diagonal matrix $S_{ij} = \sqrt{m_{ii}}\delta_{ij}$ and new coordinates $y_i = S_{ii}x_i = \sum_j S_{ij}x_j$, or $y = S \cdot x$. Now $m = S^2 = S^T \cdot S$, so $T = \frac{1}{2}\dot{x}^T \cdot m \cdot \dot{x} = \frac{1}{2}\dot{x}^T \cdot S^T \cdot S \cdot \dot{x} = \frac{1}{2}\left(S \cdot \dot{x}\right)^T \cdot S \cdot \dot{x} = \frac{1}{2}\dot{y}^T \cdot \dot{y}$. In terms of y, the potential energy is $U = \frac{1}{2}y^T \cdot B \cdot y$, where

$$B = S^{-1} \cdot \mathcal{O}_1 \cdot A \cdot \mathcal{O}_1^{-1} \cdot S^{-1}$$

is still a symmetric matrix.

Finally, let $\mathcal{O}_2$ be an orthogonal matrix which diagonalizes B, so $C = \mathcal{O}_2 \cdot B \cdot \mathcal{O}_2^{-1}$ is diagonal, and let $\xi = \mathcal{O}_2 \cdot y$. Just as in the first step,

$$U = \frac{1}{2}\xi^T \cdot \mathcal{O}_2 \cdot B \cdot \mathcal{O}_2^{-1} \cdot \xi = \frac{1}{2}\xi^T \cdot C \cdot \xi,$$

while the kinetic energy

$$T = \frac{1}{2}\dot{y}^T \cdot \dot{y} = \frac{1}{2}\dot{y}^T \cdot \mathcal{O}_2^T \cdot \mathcal{O}_2 \cdot \dot{y} = \frac{1}{2}\dot{\xi}^T \cdot \dot{\xi}$$

is still diagonal. Because the potential energy must still be nonnegative, all the diagonal elements C_{ii} are nonnegative, and we will call them $\omega_i := \sqrt{C_{ii}}$. Then

$$T = \frac{1}{2}\sum_j \dot{\xi}_j^2, \qquad U = \frac{1}{2}\sum_j \omega_j^2 \xi_j^2, \qquad \ddot{\xi}_j + \omega_j^2 \xi_j = 0,$$

so we have N independent harmonic oscillators with the solutions

$$\xi_j = \text{ Re } a_j e^{i\omega_j t},$$

with some arbitrary complex numbers a_j.

To find what the solution looks like in terms of the original coordinates q_i, we need to undo all these transformations. As $\xi = \mathcal{O}_2 \cdot y = \mathcal{O}_2 \cdot S \cdot x = \mathcal{O}_2 \cdot S \cdot \mathcal{O}_1 \cdot \eta$, we have

$$q = q_0 + \mathcal{O}_1^{-1} \cdot S^{-1} \cdot \mathcal{O}_2^{-1} \cdot \xi.$$

We have completely solved this very general problem in small oscillations, at least in the sense that we have reduced it to a solvable problem of diagonalizing symmetric real matrices. What we have done may appear abstract and formal and devoid of physical insight, but it is a general algorithm which *will work* on a very wide class of problems of small oscillations about equilibrium. In fact, because diagonalizing matrices is something for which computer programs are available, this is even a practical method for solving such systems, even if there are dozens of interacting particles.

5.1.1 Molecular Vibrations

Consider a molecule made up of n atoms. We need to choose the right level of description to understand low energy excitations. We do not want to describe the molecule in terms of quarks, gluons, and leptons. Nor do we need to consider all the electronic motion, which is governed by quantum mechanics. The description we will use, called the

Born-Oppenheimer approximation, is to model the nuclei as classical particles. The electrons, which are much lighter, move around much more quickly and cannot be treated classically; we assume that for any given configuration of the nuclei, the electrons will almost instantaneously find a quantum-mechanical ground state, which will have an energy which depends on the current positions of the nuclei. This is then a potential energy when considering the nuclear motion. The nuclei themselves will be considered point particles, and we will ignore internal quantum-mechanical degrees of freedom such as nuclear spins. So we are considering n point particles moving in three dimensions, with some potential about which we know only qualitative features. There are $3n$ degrees of freedom. Of these, 3 are the center of mass motion, which, as there are no external forces, is simply motion at constant velocity. Some of the degrees of freedom describe rotational modes, *i.e.* motions that the molecule could have as a rigid body. For a generic molecule this would be three degrees of freedom, but if the equilibrium configuration of the molecule is linear, rotation about that line is not a degree of freedom, and so only two of the degrees of freedom are rotations in that case. The remaining degrees of freedom, $3n-6$ for noncollinear and $3n-5$ for collinear molecules, are **vibrations**.

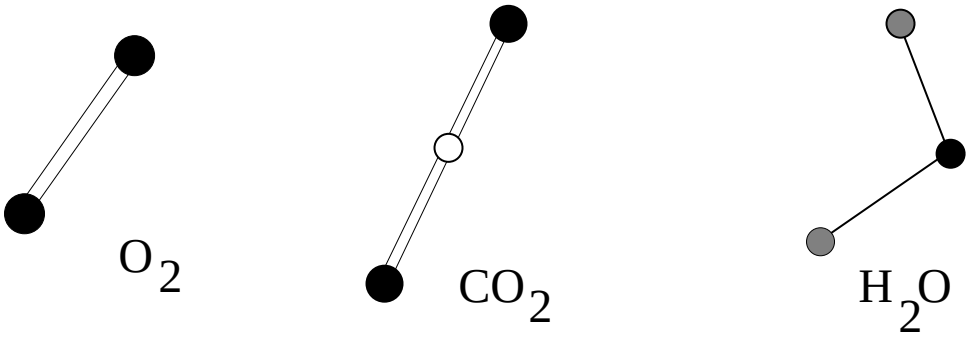


Figure 5.1: Some simple molecules in their equilibrium positions.

For a collinear molecule, it makes sense to divide the vibrations into transverse and longitudinal ones. Considering motion in one dimension only, the nuclei have n degrees of freedom, one of which is a center-of-mass motion, leaving $n-1$ longitudinal vibrations. So the remaining $(3n-5)-(n-1) = 2(n-2)$ vibrational degrees of freedom are transverse

vibrational modes. There are no such modes for a diatomic molecule.

Example: CO_2

Consider first the CO_2 molecule. As it is a molecule, there must be a position of stable equilibrium, and empirically we know it to be collinear and symmetric, which one might have guessed. We will first consider only collinear motions of the molecule. If the oxygens have coordinates q_1 and q_2, and the carbon q_3, the potential depends on q_1-q_3 and q_2-q_3 in the same way, so the equilibrium positions have $q_2-q_3 = -(q_1-q_3) = b$. Assuming no direct force between the two oxygen molecules, the one dimensional motion may be described near equilibrium by

$$\begin{aligned} U &= \frac{1}{2}k(q_3 - q_1 - b)^2 + \frac{1}{2}k(q_2 - q_3 - b)^2 \\ T &= \frac{1}{2}m_O\dot{q}_1^2 + \frac{1}{2}m_O\dot{q}_2^2 + \frac{1}{2}m_C\dot{q}_3^2. \end{aligned}$$

We gave our formal solution in terms of displacements from *the* equilibrium position, but we now have a situation in which there is no single equilibrium position, as the problem is translationally invariant, and while equilibrium has constraints on the differences of q's, there is no constraint on the center of mass. We can treat this in two different ways:

1. Explicitly fix the center of mass, eliminating one of the degrees of freedom.

2. Pick arbitrarily *an* equilibrium position. While the deviations of the center-of-mass position from the equilibrium is not confined to small excursions, the quadratic approximation is still exact.

First we follow the first method. We can always work in a frame where the center of mass is at rest, at the origin. Then $m_O(q_1 + q_2) + m_C q_3 = 0$ is a constraint, which we must eliminate. We can do so by dropping q_3 as an independant degree of freedom, and we have, in terms of the two displacements from equilibrium $\eta_1 = q_1 + b$ and $\eta_2 = q_2 - b$, $q_3 = -(\eta_1 + \eta_2)m_O/m_C$, and

$$T = \frac{1}{2}m_O(\dot{\eta}_1^2 + \dot{\eta}_2^2) + \frac{1}{2}m_C\dot{\eta}_3^2 = \frac{1}{2}m_O\left[\dot{\eta}_1^2 + \dot{\eta}_2^2 + \frac{m_O}{m_C}(\dot{\eta}_1 + \dot{\eta}_2)^2\right]$$

$$= \frac{1}{2}\frac{m_O^2}{m_C}\begin{pmatrix}\dot\eta_1 & \dot\eta_2\end{pmatrix}\begin{pmatrix}1+m_C/m_O & 1\\ 1 & 1+m_C/m_O\end{pmatrix}\begin{pmatrix}\dot\eta_1\\ \dot\eta_2\end{pmatrix}.$$

Now T is not diagonal, or more precisely M isn't. We must find the orthogonal matrix $\mathcal{O}_1$ such that $\mathcal{O}_1 \cdot M \cdot \mathcal{O}_1^{-1}$ is diagonal. We may assume it to be a rotation, which can only be

$$\mathcal{O} = \begin{pmatrix}\cos\theta & -\sin\theta\\ \sin\theta & \cos\theta\end{pmatrix}$$

for some value of θ. It is worthwhile to derive a formula for diagonalizing a general real symmetric 2×2 matrix and then plug in our particular form. Let

$$M = \begin{pmatrix}a & b\\ b & d\end{pmatrix}, \qquad \text{and} \quad \mathcal{O} = \begin{pmatrix}c & -s\\ s & c\end{pmatrix},$$

where we have abbreviated $s = \sin\theta, c = \cos\theta$. We will require the matrix element $m_{12} = (\mathcal{O}\cdot M\cdot \mathcal{O}^{-1})_{12} = 0$, because m is diagonal. This determines θ:

$$\begin{aligned}\mathcal{O}\cdot M\cdot\mathcal{O}^{-1} &= \begin{pmatrix}c & -s\\ s & c\end{pmatrix}\begin{pmatrix}a & b\\ b & d\end{pmatrix}\begin{pmatrix}c & s\\ -s & c\end{pmatrix}\\ &= \begin{pmatrix}c & -s\\ s & c\end{pmatrix}\begin{pmatrix}\cdot & as+bc\\ \cdot & bs+cd\end{pmatrix} = \begin{pmatrix}\cdot & acs+bc^2-bs^2-scd\\ \cdot & \cdot\end{pmatrix}\end{aligned}$$

where we have placed a $\cdot$ in place of matrix elements we don't need to calculate. Thus the condition on θ is

$$(a-d)\sin\theta\cos\theta + b(\cos^2\theta - \sin^2\theta) = 0 = (a-d)\sin 2\theta/2 + b\cos 2\theta,$$

or

$$\tan 2\theta = \frac{-2b}{a-d}.$$

Notice this determines 2θ only modulo π, and therefore θ modulo 90°, which ought to be expected, as a rotation through 90° only interchanges axes and reverses directions, both of which leave a diagonal matrix diagonal.

In our case $a = d$, so $\tan 2\theta = \infty$, and $\theta = \pi/4$. As $x = \mathcal{O}_1\eta$,

$$\begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} \cos\pi/4 & -\sin\pi/4 \\ \sin\pi/4 & \cos\pi/4 \end{pmatrix} \begin{pmatrix} \eta_1 \\ \eta_2 \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} \eta_1 - \eta_2 \\ \eta_1 + \eta_2 \end{pmatrix},$$

and inversely

$$\begin{pmatrix} \eta_1 \\ \eta_2 \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} x_1 + x_2 \\ -x_1 + x_2 \end{pmatrix}.$$

Then

$$\begin{aligned}
T &= \frac{1}{2} m_O \left[\frac{(\dot{x}_1 + \dot{x}_2)^2}{2} + \frac{(\dot{x}_1 - \dot{x}_2)^2}{2} + \frac{m_O}{m_C} (\sqrt{2}\dot{x}_2)^2 \right] \\
&= \frac{1}{2} m_O \dot{x}_1^2 + \frac{1}{2} m_O \left(1 + \frac{2m_O}{m_C} \right) \dot{x}_2^2 \\
U &= \frac{1}{2} k (q_3 - q_1 - b)^2 + \frac{1}{2} k (q_2 - q_3 - b)^2 \\
&= \frac{1}{2} k \left[\left(\eta_1 + \frac{m_O}{m_C} (\eta_1 + \eta_2) \right)^2 + \left(\eta_2 + \frac{m_O}{m_C} (\eta_1 + \eta_2) \right)^2 \right] \\
&= \frac{1}{2} k \left[\eta_1^2 + \eta_2^2 + \frac{2m_O^2}{m_C^2} (\eta_1 + \eta_2)^2 + \frac{2m_O}{m_C} (\eta_1 + \eta_2)^2 \right] \\
&= \frac{1}{2} k \left[x_1^2 + x_2^2 + \frac{4m_O}{m_C^2} (m_O + m_C) x_2^2 \right] \\
&= \frac{1}{2} k x_1^2 + \frac{1}{2} k \left(\frac{m_C + 2m_O}{m_C} \right)^2 x_2^2.
\end{aligned}$$

Thus U is already diagonal and we don't need to go through steps 2 and 3, the scaling and second orthogonalization, except to note that if we skip the scaling the angular frequencies are given by $\omega_i^2 =$ coefficient in U / coefficient in T. Thus we have one normal mode, x_1, with $\omega_1 = \sqrt{k/m_O}$, with $x_2 = 0$, $\eta_1 = -\eta_2$, $q_3 = 0$, in which the two oxygens vibrate in and out together, symmetrically about the carbon, which doesn't move. We also have another mode, x_2, with

$$\omega_2 = \sqrt{\frac{k(m_C + 2m_O)^2/m_O^2}{m_O(1 + 2m_O/m_C)}} = \sqrt{\frac{k(m_C + 2m_O)}{m_O m_C}},$$

with $x_1 = 0$, $\eta_1 = \eta_2$, in which the two oxygens move right or left together, with the carbon moving in the opposite direction.

We have successfully solved for the longitudinal vibrations by eliminating one of the degrees of freedom. Let us now try the second method, in which we choose an arbitrary equilibrium position $q_1 = -b$, $q_2 = b$, $q_3 = 0$. Then

$$\begin{aligned} T &= \frac{1}{2}m_O(\dot{\eta}_1^2 + \dot{\eta}_2^2) + \frac{1}{2}m_C\dot{\eta}_3^2 \\ U &= \frac{1}{2}k\left[(\eta_1 - \eta_3)^2 + (\eta_2 - \eta_3)^2\right]. \end{aligned}$$

T is already diagonal, so $\mathcal{O}_1 = \mathbb{1}$, $x = \eta$. In the second step S is the diagonal matrix with $S_{11} = S_{22} = \sqrt{m_O}$, $S_{33} = \sqrt{m_C}$, and $y_i = \sqrt{m_O}\eta_i$ for $i = 1, 2$, and $y_3 = \sqrt{m_C}\eta_3$. Then

$$\begin{aligned} U &= \frac{1}{2}k\left[\left(\frac{y_1}{\sqrt{m_O}} - \frac{y_3}{\sqrt{m_C}}\right)^2 + \left(\frac{y_2}{\sqrt{m_O}} - \frac{y_3}{\sqrt{m_C}}\right)^2\right] \\ &= \frac{1}{2}\frac{k}{m_O m_C}\left[m_C y_1^2 + m_C y_2^2 + 2m_O y_3^2 - 2\sqrt{m_O m_C}(y_1 + y_2)y_3\right]. \end{aligned}$$

Thus the matrix B is

$$B = \begin{pmatrix} m_C & 0 & -\sqrt{m_O m_C} \\ 0 & m_C & -\sqrt{m_O m_C} \\ -\sqrt{m_O m_C} & -\sqrt{m_O m_C} & 2m_O \end{pmatrix},$$

which is singular, as it annihilates the vector $y^T = (\sqrt{m_O}, \sqrt{m_O}, \sqrt{m_C})$, which corresponds to $\eta^T = (1, 1, 1)$, *i.e.* all the nuclei are moving by the same amount, or the molecule is translating rigidly. Thus this vector corresponds to a zero eigenvalue of U, and a harmonic oscillation of zero frequency. This is free motion[2], $\xi = \xi_0 + vt$. The other two modes can be found by diagonalizing the matrix, and will be as we found by the other method.

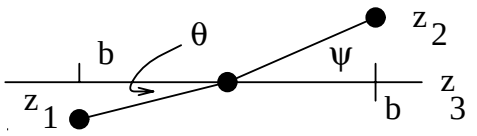
[2]To see that linear motion is a limiting case of harmonic motion as $\omega \to 0$, we need to choose the complex coefficient to be a function of ω, $A(\omega) = x_0 - iv_0/\omega$, with x_0 and v_0 real. Then $x(t) = \lim_{\omega\to 0}$ Re $A(\omega)e^{i\omega t} = x_0 + v_0 \lim_{\omega\to 0} \sin(\omega t)/\omega = x_0 + v_0 t$

Transverse motion

What about the transverse motion? Consider the equilibrium position of the molecule to lie in the x direction, and consider small deviations in the z direction. The kinetic energy

$$T = \frac{1}{2}m_O\dot{z}_1 + \frac{1}{2}m_O\dot{z}_2^2 + \frac{1}{2}m_C\dot{z}_3^2.$$

is already diagonal, just as for the longitudinal modes in the second method. Any potential energy must be due to a resistance to bending, so to second order, $U \propto (\psi - \theta)^2 \sim (\tan\psi - \tan\theta)^2 = [(z_2 - z_3)/b + (z_1 - z_3)/b]^2 = b^{-2}(z_1 + z_2 - 2z_3)^2$.



Note that the potential energy is proportional to the square of a single linear combination of the displacements, or to the square of one component (with respect to a particular direction) of the displacement. Therefore there is no contribution of the two orthogonal directions, and there are two zero modes, or two degrees of freedom with no restoring force. One of these is the center of mass motion, $z_1 = z_2 = z_3$, and the other is the third direction in the abstract space of possible displacements, $z^T = (1, -1, 0)$, with $z_1 = -z_2$, $z_3 = 0$, which we see is a rotation. Thus there remains only one true transverse vibrational mode in the z direction, and also one in the y direction, which together with the two longitudinal ones we found earlier, make up the 4 vibrational modes we expected from the general formula $2(n-2)$ for a collinear molecule.

You might ask whether these oscillations we have discussed are in any way observable. Quantum mechanically, a harmonic oscillator can only be in states with excitation energy $E = n\hbar\omega$, where $n \in \mathbb{Z}$ is an integer and $2\pi\hbar$ is Planck's constant. When molecules are in an excited state, they can emit a photon while changing to a lower energy state. The energy of the photon, which is the amount lost by the molecule, is proportional to the frequency, $\Delta E = 2\pi\hbar f$, so by measuring the wavelength of the emitted light, we can determine the vibrational frequencies of the molecules. So the calculations we have done, and many

others for which we have built the apparatus, are in fact very practical tools for molecular physics.

5.1.2 An Alternative Approach

The step by step diagonalization we just gave is not the easiest approach to solving the linear differential equation (5.3). Solutions to linear differential equations are subject to superposition, and equations with coefficients independent of time are simplified by Fourier transform, so we can express the N dimensional vector of functions $\eta_i(t)$ as

$$\eta_i(t) = \int_{-\infty}^{\infty} d\omega f_j(\omega) e^{-i\omega t}.$$

Then the Lagrange equations become

$$\int_{-\infty}^{\infty} d\omega \left(A_{ij} - \omega^2 M_{ij}\right) f_j(\omega) e^{-i\omega t} = 0 \quad \text{for all } t.$$

But $e^{-i\omega t}$ are linearly independent functions of $t \in \mathbb{R}$, so

$$\left(A_{ij} - \omega^2 M_{ij}\right) f_j(\omega) = 0.$$

This implies $f_j(\omega) = 0$ except when the matrix $A_{ij} - \omega^2 M_{ij}$ is singular, $\det\left(A_{ij} - \omega^2 M_{ij}\right) = 0$, which gives a descrete set of angular frequencies $\omega_1 \ldots \omega_N$, and for each an eigenvector f_j.

5.2 Other interactions

In our treatment we assumed a Lagrangian formulation with a kinetic term purely quadratic in $\dot{\vec{q}}$, together with a velocity independent potential. There is a wider scope of small oscillation problems which might include dissipative forces like friction, or external time-dependent forces, or perhaps terms in the Lagrangian linear in the velocities. An example of the latter occurs in rotating reference frames, from the Coriolus force, and is important in the question of whether there is a gravitationally stable location for small objects caught between the Earth and the moon at the "L5" point. Each of these complications introduces terms,

even in the linear approximation to the equations of motion, which cannot be diagonalized away, because there is not significant freedom of diagonalization left, in general, after having simplified T and U. Thus the approach of section 5.1 does not generalize well, but the approach of section 5.1.2 can be applied.

5.3 String dynamics

In this section we consider two closely related problems, transverse oscillations of a stretched loaded string, and of a stretched heavy string. The latter is is a limiting case of the former. This will provide an introduction to field theory, in which the dynamical degrees of freedom are not a discrete set but are defined at each point in space. In Chapter 8 we will discuss more interesting and involved cases such as the electromagnetic field, where at each point in space we have $\vec{E}$ and $\vec{B}$ as degrees of freedom, though not without constraints.

The loaded string we will consider is a light string under tension τ stretched between two fixed points a distance ℓ apart, say at $x = 0$ and $x = \ell$. On the string, at points $x = a, 2a, 3a, \ldots, na$, are fixed n particles each of mass m, with the first and last a distance a away from the fixed ends. Thus $\ell = (n + 1)a$. We will consider only small transverse motion of these masses, using y_i as the transverse displacement of the i'th mass, which is at $x = ia$. We assume all excursions from the equilibrium positions $y_i = 0$ are small, and in particular that the difference in successive displacements $y_{i+1} - y_i \ll a$. Thus we are assuming that the angle made by each segment of the string, $\theta_i = \tan^{-1}[(y_{i+1} - y_i)/a] \ll 1$. Working to first order in the θ's in the equations of motion, and second order for the Lagrangian, we see that restricting our attention to transverse motions and requiring no horizontal motion forces taking the tension τ to be constant along the string. The transverse force on the i'th mass is thus

$$F_i = \tau \frac{y_{i+1} - y_i}{a} + \tau \frac{y_{i-1} - y_i}{a} = \frac{\tau}{a}(y_{i+1} - 2y_i + y_{i-1}).$$

The potential energy $U(y_1, \ldots, y_n)$ then satisfies

$$\frac{\partial U}{\partial y_i} = -\frac{\tau}{a}(y_{i+1} - 2y_i + y_{i-1})$$

so

$$\begin{aligned}
&U(y_1,\ldots,y_i,\ldots,y_n)\\
&\quad=\int_0^{y_i} dy_i\,\frac{\tau}{a}(2y_i-y_{i+1}-y_{i-1})+F(y_1,\ldots,y_{i-1},y_{i+1},\ldots,y_n)\\
&\quad=\frac{\tau}{a}\left(y_i^2-(y_{i+1}+y_{i-1})y_i\right)+F(y_1,\ldots,y_{i-1},y_{i+1},\ldots,y_n)\\
&\quad=\frac{\tau}{2a}\left((y_{i+1}-y_i)^2+(y_i-y_{i-1})^2\right)+F'(y_1,\ldots,y_{i-1},y_{i+1},\ldots,y_n)\\
&\quad=\sum_{i=0}^{n}\frac{\tau}{2a}\,(y_{i+1}-y_i)^2+\text{constant}.
\end{aligned}$$

The F and F' are unspecified functions of all the y_j's except y_i. In the last expression we satisfied the condition for all i, and we have used the convenient definition $y_0 = y_{n+1} = 0$. We can and will drop the arbitrary constant.

The kinetic energy is simply $T = \frac{1}{2}m\sum_1^n \dot{y}_i^2$, so the mass matrix is already proportional to the identity matrix and we do not need to go through the first two steps of our general process. The potential energy $U = \frac{1}{2}y^T\cdot A\cdot y$ has a non-diagonal $n\times n$ matrix

$$A=-\frac{\tau}{a}\begin{pmatrix}
-2 & 1 & 0 & 0 & \cdots & 0 & 0\\
1 & -2 & 1 & 0 & \cdots & 0 & 0\\
0 & 1 & -2 & 1 & \cdots & 0 & 0\\
\vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots\\
0 & 0 & 0 & 0 & \cdots & -2 & 1\\
0 & 0 & 0 & 0 & \cdots & 1 & -2
\end{pmatrix}.$$

Diagonalizing even a 3×3 matrix is work, so an $n\times n$ matrix might seem out of the question, without some hints from the physics of the situation. In this case the hint comes in a roundabout fashion — we will first consider a limit in which $n\to\infty$, the **continuum limit**, which leads to an interesting physical situation in its own right.

Suppose we consider the loaded string problem in the limit that the spacing a becomes very small, but the number of masses m becomes large, keeping the total length ℓ of the string fixed. If at the same time we adjust the individual masses so that the mass per unit length, ρ, is fixed, our bumpy string gets smoothed out in the limit, and we

might expect that in this limit we reproduce the physical problem of transverse modes of a uniformly dense stretched string, like a violin string. Thus we wish to consider the limit

$$a \to 0, \quad n \to \infty, \quad \ell = (n+1)a \text{ fixed}, \quad m \to 0, \quad \rho = m/a \text{ fixed}.$$

It is natural to think of the degrees of freedom as associated with the label x rather than i, so we redefine the dynamical functions $\{y_j(t)\}$ as $y(x,t)$, with $y(ja,t) = y_j(t)$. While this only defines the function at discrete points in x, these are closely spaced for small a and become dense as $a \to 0$. We will assume that the function $y(x)$ is twice differentiable in the continuum limit, though we shall see that this is not the case for all possible motions of the discrete system.

What happens to the kinetic and potential energies in this limit? For the kinetic energy,

$$T = \frac{1}{2}m\sum_i \dot{y}_i^2 = \frac{1}{2}\rho\sum_i a\dot{y}^2(x_i) = \frac{1}{2}\rho\sum_i \Delta x\dot{y}^2(x_i) \to \frac{1}{2}\rho\int_0^\ell dx\,\dot{y}^2(x),$$

where the next to last expression is just the definition of a Riemann integral. For the potential energy,

$$U = \frac{\tau}{2a}\sum_i (y_{i+1}-y_i)^2 = \frac{\tau}{2}\sum_i \Delta x\left(\frac{y_{i+1}-y_i}{\Delta x}\right)^2 \to \frac{\tau}{2}\int_0^\ell dx\,\left(\frac{\partial y}{\partial x}\right)^2.$$

The equation of motion for y_i is

$$m\ddot{y}_i = \frac{\partial L}{\partial y_i} = -\frac{\partial U}{\partial y_i} = \frac{\tau}{a}[(y_{i+1}-y_i)-(y_i-y_{i-1})],$$

or

$$\rho a\ddot{y}(x) = \frac{\tau}{a}([y(x+a)-y(x)]-[y(x)-y_(x-a)]).$$

We need to be careful about taking the limit

$$\frac{y(x+a)-y(x)}{a} \to \frac{\partial y}{\partial x}$$

because we are subtracting two such expressions evaluated at nearby points, and because we will need to divide by a again to get an equation between finite quantities. Thus we note that

$$\frac{y(x+a)-y(x)}{a} = \left.\frac{\partial y}{\partial x}\right|_{x+a/2} + \mathcal{O}(a^2),$$

so

$$\begin{aligned}\rho\ddot{y}(x) &= \frac{\tau}{a}\left(\frac{y(x+a)-y(x)}{a}-\frac{y(x)-y_(x-a)}{a}\right)\\ &\approx \frac{\tau}{a}\left(\left.\frac{\partial y}{\partial x}\right|_{x+a/2}-\left.\frac{\partial y}{\partial x}\right|_{x-a/2}\right)\to\tau\frac{\partial^2 y}{\partial x^2},\end{aligned}$$

and we wind up with the wave equation for transverse waves on a massive string

$$\frac{\partial^2 y}{\partial t^2}-c^2\frac{\partial^2 y}{\partial x^2}=0,$$

where

$$c=\sqrt{\frac{\tau}{\rho}}.$$

Solving this wave equation is very simple. For the fixed boundary conditions $y(x)=0$ at $x=0$ and $x=\ell$, the solution is a fourier expansion

$$y(x,t)=\sum_{p=1}^{\infty}\ \mathrm{Re}\ B_p e^{ick_p t}\sin k_p x,$$

where $k_p\ell = p\pi$. Each p represents one normal mode, and there are an infinite number as we would expect because in the continuum limit there are an infinite number of degrees of freedom.

We have certainly not shown that $y(x)=B\sin kx$ is a normal mode for the problem with finite n, but it is worth checking it out. This corresponds to a mode with $y_j = B\sin kaj$, on which we apply the matrix A

$$\begin{aligned}(A\cdot y)_i &= \sum_j A_{ij}y_j = -\frac{\tau}{a}\left(y_{i+1}-2y_i+y_{i-1}\right)\\ &= -\frac{\tau}{a}B\left(\sin(kai+ka)-2\sin(kai)+\sin(kai-ka)\right)\\ &= -\frac{\tau}{a}B(\sin(kai)\cos(ka)+\cos(kai)\sin(ka)-2\sin(kai)\\ &\qquad +\sin(kai)\cos(ka)-\cos(kai)\sin(ka))\\ &= \frac{\tau}{a}B\left(2-2\cos(ka)\right)\sin(kai)\\ &= \frac{2\tau}{a}\left(1-\cos(ka)\right)y_i.\end{aligned}$$

So we see that it *is* a normal mode, although the frequency of oscillation

$$\omega = \sqrt{\frac{2\tau}{am}(1-\cos(ka))} = 2\sqrt{\frac{\tau}{\rho}}\frac{\sin(ka/2)}{a}$$

differs from $k\sqrt{\tau/\rho}$ except in the limit $a \to 0$ for fixed k.

The k's which index the normal modes are restricted by the fixed ends to the discrete set $k = p\pi/\ell = p\pi/(n+1)a$, but this is still too many (∞) for a system with a finite number of degrees of freedom. The resolution of this paradox is that not all different k's correspond to different modes. For example, if $p' = p + 2m(n+1)$ for some integer m, then $k' = k + 2\pi m/a$, and $\sin(k'aj) = \sin(kaj + 2m\pi) = \sin(kaj)$, so k and k' represent the same normal mode. Also, if $p' = 2(n+1) - p$, $k' = (2\pi/a) - k$, $\sin(k'aj) = \sin(2\pi - kaj) = -\sin(kaj)$, so k and k' represent the same normal mode, with opposite phase. Finally $p = n+1$, $k = \pi/a$ gives $y_j = B\sin(kaj) = 0$ for all j and is not a normal mode. This leaves as independent only $p = 1, ..., n$, the right number of normal modes for a system with n degrees of freedom.

The angular frequency of the p'th normal mode

$$\omega_p = 2\sqrt{\frac{\tau}{ma}}\sin\frac{p\pi}{2(n+1)}$$

in plotted in Fig. 5.3. For fixed values of p and ρ, as $n \to \infty$,

$$\omega_p = 2\sqrt{\frac{\tau}{\rho}}\frac{1}{a}\sin\frac{pa\pi}{2\ell} \to 2\sqrt{\frac{\tau}{\rho}}\frac{p\pi}{2\ell} = ck_p,$$

as we have in the continuum limit. But if we consider modes with a fixed ratio of p/n as $n \to \infty$, we do not have a smooth limit $y(x)$, and such nodes are not appropriate for the continuum limit. In the physics of crystals, the former kind of modes are known as **accoustic modes**, while the later modes, in particular those for $n - p$ fixed, which depend on the discrete nature of the crystal, are called **optical modes**.

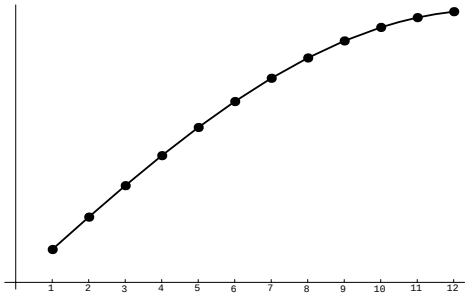


Fig. 5.3. Frequencies of oscillation of the loaded string.

5.4 Field theory

We saw in the last section that the kinetic and potential energies in the continuum limit can be written as integrals over x of densities, and so we may also write the Lagrangian as the integral of a **Lagrangian density** $\mathcal{L}(x)$,

$$L = T - U = \int_0^L dx \mathcal{L}(x), \qquad \mathcal{L}(x) = \left[\frac{1}{2}\rho \dot{y}^2(x,t) - \frac{1}{2}\tau \left(\frac{\partial y(x,t)}{\partial x} \right)^2 \right].$$

This Lagrangian, however, will not be of much use until we figure out what is meant by varying it with respect to each dynamical degree of freedom or its corresponding velocity. In the discrete case we have the canonical momenta $P_i = \partial L/\partial \dot{y}_i$, where the derivative requires holding all $\dot{y}_j$ fixed, for $j \neq i$, as well as all y_k fixed. This extracts one term from the sum $\frac{1}{2}\rho \sum a \dot{y}_i^2$, and this would appear to vanish in the limit $a \to 0$. Instead, we define the canonical momentum as a density, $P_i \to aP(x = ia)$, so

$$P(x = ia) = \lim \frac{1}{a} \frac{\partial}{\partial \dot{y}_i} \sum_i a \, \mathcal{L}(y(x), \dot{y}(x), x)\big|_{x=ai} .$$

We may think of the last part of this limit,

$$\lim_{a\to 0}\sum_i a\,\mathcal{L}(y(x),\dot{y}(x),x)|_{x=ai} = \int dx\,\mathcal{L}(y(x),\dot{y}(x),x),$$

if we also define a limiting operation

$$\lim_{a\to 0}\frac{1}{a}\frac{\partial}{\partial\dot{y}_i}\to\frac{\delta}{\delta\dot{y}(x)},$$

and similarly for $\frac{1}{a}\frac{\partial}{\partial y_i}$, which act on functionals of $y(x)$ and $\dot{y}(x)$ by

$$\frac{\delta y(x_1)}{\delta y(x_2)}=\delta(x_1-x_2),\quad \frac{\delta\dot{y}(x_1)}{\delta y(x_2)}=\frac{\delta y(x_1)}{\delta\dot{y}(x_2)}=0,\quad \frac{\delta\dot{y}(x_1)}{\delta\dot{y}(x_2)}=\delta(x_1-x_2).$$

Here $\delta(x'-x)$ is the **Dirac delta function**, defined by its integral,

$$\int_{x_1}^{x_2} f(x')\delta(x'-x)dx' = f(x)$$

for any function $f(x)$, provided $x\in(x_1,x_2)$. Thus

$$P(x)=\frac{\delta}{\delta\dot{y}(x)}\int_0^\ell dx'\frac{1}{2}\rho\dot{y}^2(x',t)=\int_0^\ell dx'\rho\dot{y}(x',t)\delta(x'-x)=\rho\dot{y}(x,t).$$

We also need to evaluate

$$\frac{\delta}{\delta y(x)}L=\frac{\delta}{\delta y(x)}\int_0^\ell dx'\frac{-\tau}{2}\left(\frac{\partial y}{\partial x}\right)^2_{x=x'}.$$

For this we need

$$\frac{\delta}{\delta y(x)}\frac{\partial y(x')}{\partial x'}=\frac{\partial}{\partial x'}\delta(x'-x):=\delta'(x'-x),$$

which is again defined by its integral,

$$\begin{aligned}\int_{x_1}^{x_2} f(x')\delta'(x'-x)dx' &= \int_{x_1}^{x_2} f(x')\frac{\partial}{\partial x'}\delta(x'-x)dx'\\ &= f(x')\delta(x'-x)|_{x_1}^{x_2}-\int_{x_1}^{x_2}dx'\,\frac{\partial f}{\partial x'}\delta(x'-x)\\ &= \frac{\partial f}{\partial x}(x),\end{aligned}$$

where after integration by parts the surface term is dropped because $\delta(x-x')=0$ for $x \neq x'$, which it is for $x'=x_1, x_2$ if $x \in (x_1, x_2)$. Thus

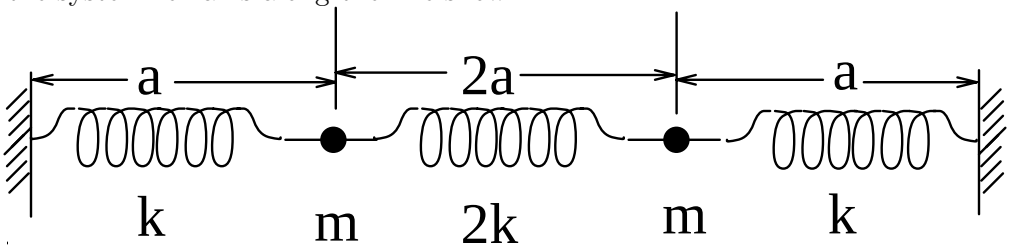
$$\frac{\delta}{\delta y(x)} L = -\int_0^\ell dx' \tau \frac{\partial y}{\partial x}(x') \delta'(x'-x) = \tau \frac{\partial^2 y}{\partial x^2},$$

and Lagrange's equations give the wave equation

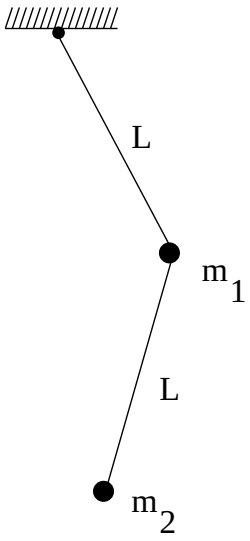
$$\rho \ddot{y}(x,t) - \tau \frac{\partial^2 y}{\partial x^2} = 0.$$

Exercises

5.1 Three springs connect two masses to each other and to immobile walls, as shown. Find the normal modes and frequencies of oscillation, assuming the system remains along the line shown.



5.2 Consider the motion, in a vertical plane of a double pendulum consisting of two masses attached to each other and to a fixed point by inextensible strings of length L. The upper mass has mass m_1 and the lower mass m_2. This is all in a laboratory with the ordinary gravitational forces near the surface of the Earth.



a) Set up the Lagrangian for the motion, assuming the strings stay taut.
b) Simplify the system under the approximation that the motion involves only small deviations from equilibrium. Put the problem in matrix form appropriate for the procedure discussed in class.
c) Find the frequencies of the normal modes of oscillation. [Hint: following exactly the steps given in class will be complex, but the analogous procedure reversing the order of U and T will work easily.]

5.3 (a) Show that if three mutually gravitating point masses are at the vertices of an equilateral triangle which is rotating about an axis normal to the plane of the triangle and through the center of mass, at a suitable angular velocity ω, this motion satisfies the equations of motion. Thus this configuration is an equilibrium in the rotating coordinate system. Do not assume the masses are equal.
(b) Suppose that two stars of masses M_1 and M_2 are rotating in circular orbits about their common center of mass. Consider a small mass m which is approximately in the equilibrium position described above (which is known as the L_5 point). The mass is small enough that you can ignore its effect on the two stars. Analyze the motion, considering specifically the stability of the equilibrium point as a function of the ratio of the masses of the stars.

Chapter 6

Hamilton's Equations

We discussed the generalized momenta

$$p_i = \frac{\partial L(q, \dot{q}, t)}{\partial \dot{q}_i},$$

and how the canonical variables $\{q_i, p_j\}$ describe phase space. One can use phase space rather than $\{q_i, \dot{q}_j\}$ to describe the state of a system at any moment. In this chapter we will explore the tools which stem from this phase space approach to dynamics.

6.1 Legendre transforms

The important object for determining the motion of a system using the Lagrangian approach is not the Lagrangian itself but its variation, under arbitrary changes in the variables q and $\dot{q}$, treated as independent variables. It is the vanishing of the variation of the action under such variations which determines the dynamical equations. In the phase space approach, we want to change variables $\dot{q} \to p$, where the p_i are part of the gradient of the Lagrangian with respect to the velocities. This is an example of a general procedure called the Legendre transformation. We will discuss it in terms of the mathematical concept of a differential form.

Because it is the variation of L which is important, we need to focus our attention on the differential dL rather than on L itself. We first

want to give a formal definition of the differential, which we will do first for a function $f(x_1, ..., x_n)$ of n variables, although for the Lagrangian we will later subdivide these into coordinates and velocities. We will take the space in which x takes values to be some general space we call $\mathcal{M}$, which might be ordinary Euclidean space but might be something else, like the surface of a sphere[1]. Given a function f of n independent variables x_i, the differential is

$$df = \sum_{i=1}^{n} \frac{\partial f}{\partial x_i} dx_i. \tag{6.1}$$

What does that mean? As an approximate statement, this can be regarded as saying

$$df \approx \Delta f \equiv f(x_i + \Delta x_i) - f(x_i) = \sum_{i=1}^{n} \frac{\partial f}{\partial x_i} \Delta x_i + \mathcal{O}(\Delta x_i \Delta x_j),$$

with some statement about the Δx_i being small, followed by the dropping of the "order $(\Delta x)^2$" terms. Notice that df is a function not only of the point $x \in \mathcal{M}$, but also of the small displacements Δx_i. A very useful mathematical language emerges if we formalize the definition of df, extending its definition to arbitrary Δx_i, even when the Δx_i are not small. Of course, for large Δx_i they can no longer be thought of as the difference of two positions in $\mathcal{M}$ and df no longer has the meaning of the difference of two values of f. Our formal df is now defined as a linear function of these Δx_i variables, which we therefore consider to be a vector $\vec{v}$ lying in an n-dimensional vector space $\mathbb{R}^n$. Thus $df : \mathcal{M} \times \mathbb{R}^n \to \mathbb{R}$ is a real-valued function with two arguments, one in $\mathcal{M}$ and one in a vector space. The dx_i which appear in (6.1) can be thought of as operators acting on this vector space argument to extract the $i'th$ component, and the action of df on the argument $(x, \vec{v})$ is $df(x, \vec{v}) = \sum_i (\partial f / \partial x_i) v_i$.

This differential is a special case of a 1-form, as is each of the operators dx_i. All n of these dx_i form a basis of **1-forms**, which are more generally

$$\omega = \sum_i \omega_i(x) dx^i.$$

[1]Mathematically, $\mathcal{M}$ is a manifold, but we will not carefully define that here. The precise definition is available in Ref. [11].

If there exists an ordinary function $f(x)$ such that $\omega = df$, then ω is said to be an **exact** 1-form.

Consider $L(q_i, v_j, t)$, where $v_i = \dot{q}_i$. At a given time we consider q and v as independant variables. The differential of L on the space of coordinates and velocities, at a fixed time, is

$$dL = \sum_i \frac{\partial L}{\partial q_i} dq_i + \sum_i \frac{\partial L}{\partial v_i} dv_i = \sum_i \frac{\partial L}{\partial q_i} dq_i + \sum_i p_i dv_i.$$

If we wish to describe physics in phase space (q_i, p_i), we are making a change of variables from v_i to the gradient with respect to these variables, $p_i = \partial L/\partial v_i$, where we focus now on the variables being transformed and ignore the fixed q_i variables. So $dL = \sum_i p_i dv_i$, and the p_i are functions of the v_j determined by the function $L(v_i)$. Is there a function $g(p_i)$ which reverses the roles of v and p, for which $dg = \sum_i v_i dp_i$? If we can invert the functions $p(v)$, we can define $g(p_i) = \sum_i v_i p_i - L(v_i(p_j))$, which has a differential

$$\begin{aligned} dg &= \sum_i dv_i p_i + \sum_i v_i dp_i - dL = \sum_i dv_i p_i + \sum_i v_i dp_i - \sum_i p_i dv_i \\ &= \sum_i v_i dp_i \end{aligned}$$

as requested, and which also determines the relationship between v and p,

$$v_i = \frac{\partial g}{\partial p_i} = v_i(p_j),$$

giving the inverse relation to $p_k(v_\ell)$. This particular form of changing variables is called a **Legendre transformation**. In the case of interest here, the function g is called $H(q_i, p_j, t)$, the **Hamiltonian**,

$$H = \sum_i \dot{q}_i p_i - L. \tag{6.2}$$

Other examples of Legendre transformations occur in thermodynamics. The energy change of a gas in a variable container with heat flow is sometimes written

$$dE = đQ - pdV,$$

where đQ is not an exact differential, and the heat Q is not a well defined system variable. Instead one defines the entropy and temperature đ$Q = TdS$, and the entropy S is a well defined property of the gas. Thus the state of the gas can be described by the two variables S and V, and changes involve an energy change

$$dE = TdS - pdV.$$

We see that the temperature is $T = \partial E/\partial S|_V$. If we wish to find quantities appropriate for describing the gas as a function of T rather than S, we define the **free energy** F by $-F = TS - E$ so $dF = -SdT - pdV$, and we treat F as a function $F(T, V)$. Alternatively, to use the pressure p rather than V, we define the **enthalpy** $X(p, S) = Vp + E$, $dX = Vdp + TdS$. To make both changes, and use (T, p) to describe the state of the gas, we use the **Gibbs free energy** $G(T, p) = X - TS = E + Vp - TS$, $dG = Vdp - SdT$

Most Lagrangians we encounter have the decomposition $L = L_2 + L_1 + L_0$ into terms quadratic, linear, and independent of velocities, as considered in 2.1.5. Then the momenta are linear in velocities, $p_i = \sum_j M_{ij}\dot{q}_j + a_i$, or in matrix form $p = M \cdot \dot{q} + a$, which has the inverse relation $\dot{q} = M^{-1} \cdot (p - a)$. As $H = L_2 - L_0$, $H = \frac{1}{2}(p - a) \cdot M^{-1} \cdot (p - a) - L_0$. As an example, consider spherical coordinates, in which the kinetic energy is

$$T = \frac{m}{2}\left(\dot{r}^2 + r^2\dot{\theta}^2 + r^2\sin^2\theta\dot{\phi}^2\right) = \frac{1}{2m}\left(p_r^2 + \frac{p_\theta^2}{r^2} + \frac{p_\phi^2}{r^2\sin^2\theta}\right).$$

Note that $p_\theta \neq \vec{p} \cdot \hat{e}_\theta$, in fact it doesn't even have the same units.

The equations of motion in Hamiltonian form,

$$\dot{q}_k = \left.\frac{\partial H}{\partial p_k}\right|_{q,t}, \qquad \dot{p}_k = -\left.\frac{\partial H}{\partial q_k}\right|_{p,t},$$

are almost symmetric in their treatment of q and p. If we define a $2N$ dimensional coordinate η for phase space,

$$\left.\begin{array}{ll} \eta_i & = q_i \\ \eta_{n+i} & = p_i \end{array}\right\} \qquad \text{for } 1 \leq i \leq N,$$

we can write Hamilton's equation in terms of a particular matrix J,

$$\dot{\eta}_j = J_{ij}\frac{\partial H}{\partial \eta_k}, \quad \text{where } J = \begin{pmatrix} 0 & \mathbb{1}_{N\times N} \\ -\mathbb{1}_{N\times N} & 0 \end{pmatrix}.$$

J is like a multidimensional version of the $i\sigma_y$ which we meet in quantum-mechanical descriptions of spin 1/2 particles. It is real, antisymmetric, and because $J^2 = -\mathbb{1}$, it is orthogonal. Mathematicians would say that J describes the **complex structure on phase space**.

For a given physical problem there is no unique set of generalized coordinates which describe it. Then transforming to the Hamiltonian may give different objects. An nice example is given in Goldstein, a mass on a spring attached to a "fixed point" which is on a truck moving at uniform velocity v_T, relative to the Earth. If we use the Earth coordinate x to describe the mass, the equilibrium position of the spring is moving in time, $x_{eq} = v_T t$, ignoring a negligible initial position. Thus $U = \frac{1}{2}k(x - v_T t)^2$, while $T = \frac{1}{2}m\dot{x}^2$ as usual, and $L = \frac{1}{2}m\dot{x}^2 - \frac{1}{2}k(x - v_T t)^2$, $p = m\dot{x}$, $H = p^2/2m + \frac{1}{2}k(x - v_T t)^2$. The equations of motion $\dot{p} = m\ddot{x} = -\partial H/\partial x = -k(x - v_T t)$, of course, show that H is not conserved, $dH/dt = (p/m)dp/dt + k(\dot{x} - v_T)(x - v_T t) = -(kp/m)(x - v_T t) + (kp/m - kv_T)(x - v_T t) = -kv_T(x - v_T t) \neq 0$. Alternatively, $dH/dt = -\partial L/\partial t = -kv_T(x - v_T t) \neq 0$. This is not surprising; the spring exerts a force on the truck and the truck is doing work to keep the fixed point moving at constant velocity.

On the other hand, if we use the truck coordinate $x' = x - v_T t$, we may describe the motion in this frame with $T' = \frac{1}{2}m\dot{x}'^2$, $U' = \frac{1}{2}kx'^2$, $L' = \frac{1}{2}m\dot{x}'^2 - \frac{1}{2}kx'^2$, giving the correct equations of motion $p' = m\dot{x}'$, $\dot{p}' = m\ddot{x}' = -\partial L'/\partial x' = -kx'$. With this set of coordinates, the Hamiltonian is $H' = \dot{x}'p' - L' = p'^2/2m + \frac{1}{2}kx'^2$, which is conserved. From the correspondence between the two sets of variables, $x' = x - v_T t$, and $p' = p - mv_T$, we see that the Hamiltonians at corresponding points in phase space differ, $H(x,p) - H'(x',p') = (p^2 - p'^2)/2m = 2mv_T p - \frac{1}{2}mv_T^2 \neq 0$.

6.2 Variations on phase curves

In applying Hamilton's Principle to derive Lagrange's Equations, we considered variations in which $\delta q_i(t)$ was arbitrary except at the initial and final times, but the velocities were fixed in terms of these, $\delta\dot{q}_i(t) = (d/dt)\delta q_i(t)$. In discussing dynamics in terms of phase space, this is not the most natural variation, because this means that the momenta are not varied independently. Here we will show that Hamilton's equations follow from a modified Hamilton's Principle, in which the momenta are freely varied.

We write the action in terms of the Hamiltonian,

$$I = \int_{t_i}^{t_f} \left[\sum_i p_i\dot{q}_i - H(q_j, p_j, t)\right] dt,$$

and consider its variation under arbitrary variation of the path in phase space, $(q_i(t), p_i(t))$. The $\dot{q}_i(t)$ is still dq_i/dt, but the momentum is varied free of any connection to $\dot{q}_i$. Then

$$\delta I = \int_{t_i}^{t_f} \left[\sum_i \delta p_i \left(\dot{q}_i - \frac{\partial H}{\partial p_i}\right) - \sum_i \delta q_i \left(\dot{p}_i + \frac{\partial H}{\partial q_i}\right)\right] dt + \sum_i p_i \delta q_i \Bigg|_{t_i}^{t_f},$$

where we have integrated the $\int \sum p_i d\delta q_i/dt$ term by parts. Note that in order to relate stationarity of the action to Hamilton Equations of Motion, it is necessary only to constrain the $q_i(t)$ at the initial and final times, without imposing any limitations on the variation of $p_i(t)$, either at the endpoints, as we did for $q_i(t)$, or in the interior (t_i, t_f), where we had previously related p_i and $\dot{q}_j$. The relation between $\dot{q}_i$ and p_j emerges instead among the equations of motion.

The $\dot{q}_i$ seems a bit out of place in a variational principle over phase space, and indeed we can rewrite the action integral as an integral of a 1-form over a path in extended phase space,

$$I = \int \sum_i p_i dq_i - H(q, p, t)dt.$$

We will see, in section 6.6, that the first term of the integrand leads to a very important form on phase space, and that the whole integrand is an important 1-form on extended phase space.

6.3 Canonical transformations

We have seen that it is often useful to switch from the original set of coordinates in which a problem appeared to a different set in which the problem became simpler. We switched from cartesian to center-of-mass spherical coordinates to discuss planetary motion, for example, or from the Earth frame to the truck frame in the example in which we found how Hamiltonians depend on coordinate choices. In all these cases we considered a change of coordinates $q \to Q$, where each Q_i is a function of all the q_j and possibly time, but not of the momenta or velocities. This is called a **point transformation**. But we have seen that we can work in phase space where coordinates and momenta enter together in similar ways, and we might ask ourselves what happens if we make a change of variables on phase space, to new variables $Q_i(q,p,t)$, $P_i(q,p,t)$. We should not expect the Hamiltonian to be the same either in form or in value, as we saw even for point transformations, but there must be a new Hamiltonian $K(Q,P,t)$ from which we can derive the correct equations of motion,

$$\dot{Q}_i = \frac{\partial K}{\partial P_i}, \qquad \dot{P}_i = -\frac{\partial K}{\partial Q_i}.$$

The analog of η for our new variables will be called ζ, so

$$\zeta = \begin{pmatrix} Q \\ P \end{pmatrix}, \qquad \dot{\zeta} = J \cdot \frac{\partial K}{\partial \zeta}.$$

If this exists, we say the new variables (Q,P) are **canonical variables** and the transformation $(q,p) \to (Q,P)$ is a **canonical transformation**.

These new Hamiltonian equations are related to the old ones, $\dot{\eta} = J \cdot \partial H/\partial \eta$, by the function which gives the new coordinates and momenta in terms of the old, $\zeta = \zeta(\eta, t)$. Then

$$\dot{\zeta}_i = \frac{d\zeta_i}{dt} = \sum_j \frac{\partial \zeta_i}{\partial \eta_j}\dot{\eta}_j + \frac{\partial \zeta_i}{\partial t}.$$

Let us write the Jacobian matrix $M_{ij} := \partial \zeta_i/\partial \eta_j$. In general, M will not be a constant but a function on phase space. The above relation

for the velocities now reads

$$\dot{\zeta} = M \cdot \dot{\eta} + \left.\frac{\partial \zeta}{\partial t}\right|_{\eta}.$$

The gradients in phase space are also related,

$$\left.\frac{\partial}{\partial \eta_i}\right|_{t,\eta} = \left.\frac{\partial \zeta_j}{\partial \eta_i}\right|_{t,\eta} \left.\frac{\partial}{\partial \zeta_j}\right|_{t,\zeta}, \quad \text{or } \nabla_\eta = M^T \cdot \nabla_\zeta.$$

Thus we have

$$\begin{aligned} \dot{\zeta} &= M \cdot \dot{\eta} + \frac{\partial \zeta}{\partial t} = M \cdot J \cdot \nabla_\eta H + \frac{\partial \zeta}{\partial t} = M \cdot J \cdot M^T \cdot \nabla_\zeta H + \frac{\partial \zeta}{\partial t} \\ &= J \cdot \nabla_\zeta K. \end{aligned}$$

Let us first consider a canonical transformation which does not depend on time, so $\left.\partial\zeta/\partial t\right|_\eta = 0$. We see that we can choose the new Hamiltonian to be the same as the old, $K = H$, and get correct mechanics, if

$$M \cdot J \cdot M^T = J. \tag{6.3}$$

We will require this condition even when ζ does depend on t, but then se need to revisit the question of finding K.

The condition (6.3) on M is similar to, and a generalization of, the condition for orthogonality of a matrix, $\mathcal{O}\mathcal{O}^T = \mathbb{1}$, which is of the same form with J replaced by $\mathbb{1}$. Another example of this kind of relation in physics occurs in special relativity, where a Lorentz transformation $L_{\mu\nu}$ gives the relation between two coordinates, $x'_\mu = \sum_\nu L_{\mu\nu} x_\nu$, with x_ν a four dimensional vector with $x_4 = ct$. Then the condition which makes L a Lorentz transformation is

$$L \cdot g \cdot L^T = g, \quad \text{with } g = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}.$$

The matrix g in relativity is known as the indefinite metric, and the condition on L is known as pseudo-orthogonality. In our main discussion, however, J is not a metric, as it is antisymmetric rather than symmetric, and the word which describes M is **symplectic**.

Just as for orthogonal transformations, symplectic transformations can be divided into those which can be generated by infinitesimal transformations (which are connected to the identity) and those which can not. Consider a transformation M which is almost the identity, $M_{ij} = \delta_{ij} + \epsilon G_{ij}$, or $M = \mathbb{1} + \epsilon G$, where ϵ is considered some infinitesimal parameter while G is a finite matrix. As M is symplectic, $(1 + \epsilon G) \cdot J \cdot (1 + \epsilon G^T) = J$, which tells us that to lowest order in ϵ, $GJ + JG^T = 0$. Comparing this to the condition for the generator of an infinitesimal rotation, $\Omega = -\Omega^T$, we see that it is similar except for the appearence of J on opposite sides, changing orthogonality to symplecticity. The new variables under such a canonical transformation are $\zeta = \eta + \epsilon G \cdot \eta$.

One important example of an infinitesimal canonical transformation is the one which relates (time dependent transformations (?)) at different times. Suppose $\eta \to \zeta(\eta, t)$ is a canonical tranformation which depends on time. One particular one is $\eta \to \zeta_0 = \zeta(\eta, t_0)$ for some particular time, so $\zeta_0 \to \zeta(\eta, t_0)$ is also a canonical transformation, and for $t = t_0 + \Delta t \approx t_0$ it will be nearly the identity if $\zeta(\eta, t)$ is differentiable.

Notice that the relationship ensuring Hamilton's equations exist,

$$M \cdot J \cdot M^T \cdot \nabla_\zeta H + \frac{\partial \zeta}{\partial t} = J \cdot \nabla_\zeta K,$$

with the symplectic condition $M \cdot J \cdot M^T = J$, implies $\nabla_\zeta (K - H) = -J \cdot \partial\zeta/\partial t$, so K differs from H here. This discussion holds as long as M is symplectic, even if it is not an infinitesimal transformation.

6.4 Poisson Brackets

Suppose I have some function $f(q, p, t)$ on phase space and I want to ask how f changes as the system evolves with time. Then

$$\begin{aligned} \frac{df}{dt} &= \sum_i \frac{\partial f}{\partial q_i}\dot{q}_i + \sum_i \frac{\partial f}{\partial p_i}\dot{p}_i + \frac{\partial f}{\partial t} \\ &= \sum_i \frac{\partial f}{\partial q_i}\frac{\partial H}{\partial p_i} - \sum_i \frac{\partial f}{\partial p_i}\frac{\partial H}{\partial q_i} + \frac{\partial f}{\partial t}. \end{aligned}$$

The structure of the first two terms is that of a **Poisson bracket**, a bilinear operation of functions on phase space defined by

$$[u, v] := \sum_i \frac{\partial u}{\partial q_i}\frac{\partial v}{\partial p_i} - \sum_i \frac{\partial u}{\partial p_i}\frac{\partial v}{\partial q_i}. \tag{6.4}$$

The Poisson bracket is a fundamental property of the phase space. In symplectic language,

$$[u, v] = \frac{\partial u}{\partial \eta_i} J_{ij} \frac{\partial v}{\partial \eta_j} = (\nabla_\eta u)^T \cdot J \cdot \nabla_\eta v. \tag{6.5}$$

If we describe the system in terms of a different set of canonical variables ζ, we should still find the function $f(t)$ changing at the same rate. We may think of u and v as functions of ζ as easily as of η, and we may ask whether $[u, v]_\zeta$ is the same as $[u, v]_\eta$. Using $\nabla_\eta = M^T \cdot \nabla_\zeta$, we have

$$\begin{aligned} [u, v]_\eta &= \left(M^T \cdot \nabla_\zeta u\right)^T \cdot J \cdot M^T \nabla_\zeta v = (\nabla_\zeta u)^T \cdot M \cdot J \cdot M^T \nabla_\zeta v \\ &= (\nabla_\zeta u)^T \cdot J \nabla_\zeta v = [u, v]_\zeta , \end{aligned}$$

so we see that the Poisson bracket is independent of the coordinatization used to describe phase space, as long as it is canonical.

The Poisson bracket plays such an important role in classical mechanics, and an even more important role in quantum mechanics, that it is worthwhile to discuss some of its abstract properties. First of all, from the definition it is obvious that it is antisymmetric:

$$[u, v] = -[v, u]. \tag{6.6}$$

It is a linear operator on each function over *constant* linear combinations, but is satisfies a Leibnitz rule for non-constant multiples,

$$[uv, w] = [u, w]v + u[v, w], \tag{6.7}$$

which follows immediately from the definition, using Leibnitz' rule on the partial derivatives. A very special relation is the **Jacobi identity**,

$$[u, [v, w]] + [v, [w, u]] + [w, [u, v]] = 0. \tag{6.8}$$

We need to prove that this is true. To simplify the presentation, we introduce some abbreviated notation. We use a subscript $_{,i}$ to indicate partial derivative with respect to η_i, so $u_{,i}$ means $\partial u/\partial\eta_i$, and $u_{,i,j}$ means $\partial(\partial u/\partial\eta_i)/\partial\eta_j$. We will assume all our functions on phase space are suitably differentiable, so $u_{,i,j} = u_{,j,i}$. We will also use the **summation convention**, that any index which appears twice in a term is assumed to be summed over[2]. Then $[v,w] = v_{,i}J_{ij}w_{,j}$, and

$$\begin{aligned}[u,[v,w]] &= [u, v_{,i}J_{ij}w_{,j}] \\ &= [u,v_{,i}]J_{ij}w_{,j} + v_{,i}J_{ij}[u,w_{,j}] \\ &= u_{,k}J_{k\ell}v_{,i,\ell}J_{ij}w_{,j} + v_{,i}J_{ij}u_{,k}J_{k\ell}w_{,j,\ell}.\end{aligned}$$

In the Jacobi identity, there are two other terms like this, one with the substitution $u \to v \to w \to u$ and the other with $u \to w \to v \to u$, giving a sum of six terms. The only ones involving second derivatives of v are the first term above and the one found from applying $u \to w \to v \to u$ to the second, $u_{,i}J_{ij}w_{,k}J_{k\ell}v_{,j,\ell}$. The indices are all dummy indices, summed over, so their names can be changed, by $i \to k \to j \to \ell \to i$, converting this term to $u_{,k}J_{k\ell}w_{,j}J_{ji}v_{,\ell,i}$. Adding the original term $u_{,k}J_{k\ell}v_{,i,\ell}J_{ij}w_{,j}$, and using $v_{,\ell,i} = v_{,i,\ell}$, gives $u_{,k}J_{k\ell}w_{,j}(J_{ji}+J_{ij})v_{,\ell,i} = 0$ because J is antisymmetric. Thus the terms in the Jacobi identity involving second derivatives of v vanish, but the same argument applies in pairs to the other terms, involving second derivatives of u or of w, so they all vanish, and the Jacobi identity is proven.

This argument can be made more elegantly if we recognize that for each function f on phase space, we may view $[f,\cdot]$ as a differential operator on functions g on phase space, mapping $g \to [f,g]$. Calling this operator D_f, we see that

$$D_f = \sum_j \left(\sum_i \frac{\partial f}{\partial \eta_i} J_{ij} \right) \frac{\partial}{\partial \eta_j},$$

which is of the general form that a differential operator has,

$$D_f = \sum_j f_j \frac{\partial}{\partial \eta_j},$$

[2]This convention of understood summation was invented by Einstein, who called it the "greatest contribution of my life".

where f_j are an arbitrary set of functions on phase space. For the Poisson bracket, the functions f_j are linear combinations of the $f_{,j}$, but $f_j \neq f_{,j}$. With this interpretation, $[f,g] = D_f g$, and $[h,[f,g]] = D_h D_f g$. Thus

$$\begin{aligned}[h,[f,g]] + [f,[g,h]] &= [h,[f,g]] - [f,[h,g]] = D_h D_f g - D_f D_h g \\ &= (D_h D_f - D_f D_h) g,\end{aligned}$$

and we see that this combination of Poisson brackets involves the commutator of differential operators. But such a commutator is always a linear differential operator itself,

$$\begin{aligned}D_h D_g &= \sum_{ij} h_i \frac{\partial}{\partial \eta_i} g_j \frac{\partial}{\partial \eta_j} = \sum_{ij} h_i \frac{\partial g_j}{\partial \eta_i} \frac{\partial}{\partial \eta_j} + \sum_{ij} h_i g_j \frac{\partial^2}{\partial \eta_i \partial \eta_j} \\ D_g D_h &= \sum_{ij} g_j \frac{\partial}{\partial \eta_j} h_i \frac{\partial}{\partial \eta_i} = \sum_{ij} g_j \frac{\partial h_i}{\partial \eta_j} \frac{\partial}{\partial \eta_i} + \sum_{ij} h_i g_j \frac{\partial^2}{\partial \eta_i \partial \eta_j}\end{aligned}$$

so in the commutator, the second derivative terms cancel, and

$$\begin{aligned}D_h D_g - D_g D_h &= \sum_{ij} h_i \frac{\partial g_j}{\partial \eta_i} \frac{\partial}{\partial \eta_j} - \sum_{ij} g_j \frac{\partial h_i}{\partial \eta_j} \frac{\partial}{\partial \eta_i} \\ &= \sum_{ij} \left(h_i \frac{\partial g_j}{\partial \eta_i} - g_i \frac{\partial h_j}{\partial \eta_i} \right) \frac{\partial}{\partial \eta_j}.\end{aligned}$$

This is just another first order differential operator, so there are no second derivatives of f left in the left side of the Jacobi identity. In fact, the identity tells us that this combination is

$$D_h D_g - D_g D_h = D_{[h,g]} \tag{6.9}$$

An antisymmetric product which obeys the Jacobi identity is what makes a Lie algebra. Lie algebras are the infinitesimal generators of Lie groups, or continuous groups, one example of which is the group of rotations $SO(3)$ which we have already considered. Notice that the "product" here is not *assosciative*, $[u,[v,w]] \neq [[u,v],w]$. In fact, the difference $[u,[v,w]] - [[u,v],w] = [u,[v,w]] + [w,[u,v]] = -[v,[w,u]]$ by

the Jacobi identity, so the Jacobi identity replaces the law of associativity in a Lie algebra.

Recall that the rate at which a function on phase space, evaluated on the system as it evolves, changes with time is

$$\frac{df}{dt} = -[H, f] + \frac{\partial f}{\partial t}, \tag{6.10}$$

where H is the Hamiltonian. The function $[f, g]$ on phase space also evolves that way, of course, so

$$\begin{aligned}
\frac{d[f,g]}{dt} &= -[H,[f,g]] + \frac{\partial [f,g]}{\partial t} \\
&= [f,[g,H]] + [g,[H,f]] + \left[\frac{\partial f}{\partial t}, g\right] + \left[f, \frac{\partial g}{\partial t}\right] \\
&= \left[f, \left(-[H,g] + \frac{\partial g}{\partial t}\right)\right] + \left[g, \left([H,f] - \frac{\partial f}{\partial t}\right)\right] \\
&= \left[f, \frac{dg}{dt}\right] - \left[g, \frac{df}{dt}\right].
\end{aligned}$$

If f and g are conserved quantities, $df/dt = dg/dt = 0$, and we have the important consequence that $d[f, g]/dt = 0$. This proves **Poisson's theorem**: The Poisson bracket of two conserved quantities is a conserved quantity.

We will now show an important theorem, known as **Liouville's theorem**, that the volume of a region of phase space is invariant under canonical transformations. This is not a volume in ordinary space, but a $2n$ dimensional volume, given by integrating the volume element $\prod_{i=1}^{2n} d\eta_i$ in the old coordinates, and by

$$\prod_{i=1}^{2n} d\zeta_i = \left|\det \frac{\partial \zeta_i}{\partial \eta_j}\right| \prod_{i=1}^{2n} d\eta_i = |\det M| \prod_{i=1}^{2n} d\eta_i$$

in the new, where we have used the fact that the change of variables requires a Jacobian in the volume element. But because $J = M \cdot J \cdot M^T$, $\det J = \det M \det J \det M^T = (\det M)^2 \det J$, and J is nonsingular, so $\det M = \pm 1$, and the volume element is unchanged.

In statistical mechanics, we generally do not know the actual state of a system, but know something about the probability that the system is in a particular region of phase space. As the transformation which maps possible values of $\eta(t_1)$ to the values into which they will evolve at time t_2 is a canonical transformation, this means that the volume of a region in phase space does not change with time, although the region itself changes. Thus the probability density, specifying the likelihood that the system is near a particular point of phase space, is invariant as we move along with the system.

6.5 Higher Differential Forms

In section 6.1 we discussed a reinterpretation of the differential df as an example of a more general differential 1-form, a map $\omega : \mathcal{M} \times \mathbb{R}^n \to \mathbb{R}$. We saw that the $\{dx_i\}$ provide a basis for these forms, so the general 1-form can be written as $\omega = \sum_i \omega_i(x)\, dx_i$. The differential df gave an example. We defined an *exact* 1-form as one which is a differential of some well-defined function f. What is the condition for a 1-form to be exact? If $\omega = \sum \omega_i dx_i$ is df, then $\omega_i = \partial f/\partial x_i = f_{,i}$, and

$$\omega_{i,j} = \frac{\partial \omega_i}{\partial x_j} = \frac{\partial^2 f}{\partial x_i \partial x_j} = \frac{\partial^2 f}{\partial x_j \partial x_i} = \omega_{j,i}.$$

Thus one *necessary* condition for ω to be exact is that the combination $\omega_{j,i} - \omega_{i,j} = 0$. We will define a 2-form to be the set of these objects which must vanish. In fact, we define a **differential k-form** to be a map

$$\omega^{(k)} : \mathcal{M} \times \underbrace{\mathbb{R}^n \times \cdots \times \mathbb{R}^n}_{k \text{ times}} \to \mathbb{R}$$

which is linear in its action on each of the $\mathbb{R}^n$ and totally antisymmetric in its action on the k copies, and is a smooth function of $x \in \mathcal{M}$. At a

given point, a basis of the k-forms is[3]

$$dx_{i_1} \wedge dx_{i_2} \wedge \cdots \wedge dx_{i_k} := \sum_{P \in S_k} (-1)^P dx_{i_{P\,1}} \otimes dx_{i_{P\,2}} \otimes \cdots \otimes dx_{i_{P\,k}}.$$

For example, in three dimensions there are three independent 2-forms at a point, $dx_1 \wedge dx_2$, $dx_1 \wedge dx_3$, and $dx_2 \wedge dx_3$, where $dx_1 \wedge dx_2 = dx_1 \otimes dx_2 - dx_2 \otimes dx_1$, which means that, acting on $\vec{u}$ and $\vec{v}$, $dx_1 \wedge dx_2(\vec{u}, \vec{v}) = u_1 v_2 - u_2 v_1$. The product $\wedge$ is called the **wedge product** or **exterior product**, and can be extended to act between k_1- and k_2-forms so that it becomes an associative distributive product. Note that this definition of a k-form agrees, for $k = 1$, with our previous definition, and for $k = 0$ tells us a 0-form is simply a function on $\mathcal{M}$. The general expression for a k-form is

$$\omega^{(k)} = \sum_{i_1 < \ldots < i_k} \omega_{i_1 \ldots i_k}(x) dx_{i_1} \wedge \cdots \wedge dx_{i_k}.$$

Let us consider some examples in three dimensional Euclidean space E^3, where there is a correspondance we can make between vectors and 1- and 2-forms. In this discussion we will not be considering how the objects change under changes in the coordinates of E^3, to which we will return later.

$k = 0$**:** As always, 0-forms are simply functions, $f(x)$, $x \in E^3$.

$k = 1$**:** A 1-form $\omega = \sum \omega_i dx_i$ can be thought of, or associated with, a vector field $\vec{A}(x) = \sum \omega_i(x) \hat{e}_i$. Note that if $\omega = df$, $\omega_i = \partial f / \partial x_i$, so $\vec{A} = \vec{\nabla} f$.

$k = 2$**:** A general two form is a sum over the three independent wedge products with independent functions $B_{12}(x), B_{13}(x), B_{23}(x)$. Let

[3]Some explanation of the mathematical symbols might be in order here. S_k is the group of permutations on k objects, and $(-1)^P$ is the **sign of the permutation** P, which is plus or minus one if the permutation can be built from an even or an odd number, respectively, of transpositions of two of the elements. The tensor product $\otimes$ of two linear operators into a field is a linear operator which acts on the product space, or in other words a bilinear operator with two arguments. Here $dx_i \otimes dx_j$ is an operator on $\mathbb{R}^n \times \mathbb{R}^n$ which maps the pair of vectors $(\vec{u}, \vec{v})$ to $u_i v_j$.

us extend the definition of B_{ij} to make it an antisymmetric matrix, so

$$B = \sum_{i<j} B_{ij} dx_i \wedge dx_j = \sum_{i,j} B_{ij} dx_i \otimes dx_j.$$

As we did for the angular velocity matrix Ω in (4.2), we can condense the information in the antisymmetric matrix B_{ij} into a vector field $\vec{B} = \sum B_i \hat{e}_i$, with $B_{ij} = \sum \epsilon_{ijk} B_k$. Note that this step requires that we are working in E^3 rather than some other dimension. Thus $B = \sum_{ijk} \epsilon_{ijk} B_k dx_i \otimes dx_j$.

$k = 3$**:** There is only one basis 3-form available in three dimensions, $dx_1 \wedge dx_2 \wedge dx_3$. Any other 3-form is proportional to this one, and in particular $dx_i \wedge dx_j \wedge dx_k = \epsilon_{ijk} dx_1 \wedge dx_2 \wedge dx_3$. The most general 3-form C is simply specified by an ordinary function $C(x)$, which multiplies $dx_1 \wedge dx_2 \wedge dx_3$.

Having established, in three dimensions, a correspondance between vectors and 1- and 2-forms, and between functions and 0- and 3-forms, we can ask to what the wedge product corresponds in terms of these vectors. If $\vec{A}$ and $\vec{C}$ are two vectors corresponding to the 1-forms $A = \sum A_i dx_i$ and $C = \sum C_i dx_i$, and if $B = A \wedge C$, then

$$B = \sum_{ij} A_i C_j dx_i \wedge dx_j = \sum_{ij} (A_i C_j - A_j C_i) dx_i \otimes dx_j = \sum_{ij} B_{ij} dx_i \otimes dx_j,$$

so $B_{ij} = A_i C_j - A_j C_i$, and

$$B_k = \frac{1}{2} \sum \epsilon_{kij} B_{ij} = \frac{1}{2} \sum \epsilon_{kij} A_i C_j - \frac{1}{2} \sum \epsilon_{kij} A_j C_i = \sum \epsilon_{kij} A_i C_j,$$

so

$$\vec{B} = \vec{A} \times \vec{C},$$

and the wedge product of two 1-forms is the cross product of their vectors.

If A is a 1-form and B is a 2-form, the wedge product $C = A \wedge B = C(x) dx_1 \wedge dx_2 \wedge dx_3$ is given by

$$C \;=\; A \wedge B = \sum_i \sum_{j<k} A_i \underbrace{B_{jk}}_{\epsilon_{jk\ell} B_\ell} \underbrace{dx_i \wedge dx_j \wedge dx_k}_{\epsilon_{ijk} dx_1 \wedge dx_2 \wedge dx_3}$$

$$
\begin{aligned}
&= \sum_{i\ell} A_i B_\ell \sum_{j<k} \underbrace{\epsilon_{jk\ell}\epsilon_{ijk}}_{\text{symmetric under } j \leftrightarrow k} dx_1 \wedge dx_2 \wedge dx_3 \\
&= \frac{1}{2}\sum_{i\ell} A_i B_\ell \sum_{jk} \epsilon_{jk\ell}\epsilon_{ijk} dx_1 \wedge dx_2 \wedge dx_3 = \sum_{i\ell} A_i B_\ell \delta_{i\ell} dx_1 \wedge dx_2 \wedge dx_3 \\
&= \vec{A}\cdot\vec{B} dx_1 \wedge dx_2 \wedge dx_3,
\end{aligned}
$$

so we see that the wedge product of a 1-form and a 2-form gives the dot product of their vectors.

The exterior derivative

We defined the differential of a function f, which we now call a 0-form, giving a 1-form $df = \sum f_{,i} dx_i$. Now we want to generalize the notion of differential so that d can act on k-forms for arbitrary k. This generalized differential

$$d : k\text{-forms} \to (k+1)\text{-forms}$$

is called the **exterior derivative**. It is defined to be linear and to act on one term in the sum over basis elements by

$$
\begin{aligned}
d\left(f_{i_1\ldots i_k}(x) dx_{i_1} \wedge \cdots \wedge dx_{i_k}\right) &= \left(df_{i_1\ldots i_k}(x)\right) \wedge dx_{i_1} \wedge \cdots \wedge dx_{i_k} \\
&= \sum_j f_{i_1\ldots i_k, j} dx_j \wedge dx_{i_1} \wedge \cdots \wedge dx_{i_k}.
\end{aligned}
$$

Clearly some examples are called for, so let us look again at three dimensional Euclidean space.

$k = 0$: For a 0-form f, $df = \sum f_{,i} dx_i$, as we defined earlier. In terms of vectors, $df \sim \vec{\nabla} f$.

$k = 1$: For a 1-form $\omega = \sum \omega_i\, dx_i$, $d\omega = \sum_i d\omega_i \wedge dx_i = \sum_{ij} \omega_{i,j} dx_j \wedge dx_i = \sum_{ij} (\omega_{j,i} - \omega_{i,j})\, dx_i \otimes dx_j$, corresponding to a two form with $B_{ij} = \omega_{j,i} - \omega_{i,j}$. These B_{ij} are exactly the things which must vanish if ω is to be exact. In three dimensional Euclidean space, we have a vector $\vec{B}$ with components $B_k = \frac{1}{2}\sum \epsilon_{kij}(\omega_{j,i} - \omega_{i,j}) = \sum \epsilon_{kij}\partial_i \omega_j = (\vec{\nabla} \times \vec{\omega})_k$, so here the exterior derivative of a 1-form gives a curl, $\vec{B} = \vec{\nabla} \times \vec{\omega}$.

$k = 2$**:** On a two form $B = \sum_{i<j} B_{ij} dx_i \wedge dx_j$, the exterior derivative gives a 3-form $C = dB = \sum_k \sum_{i<j} B_{ij,k} dx_k \wedge dx_i \wedge dx_j$. In three-dimensional Euclidean space, this reduces to

$$C = \sum_{k\ell} \sum_{i<j} \left(\partial_k \epsilon_{ij\ell} B_\ell\right) \epsilon_{kij} dx_1 \wedge dx_2 \wedge dx_3 = \sum_k \partial_k B_k dx_1 \wedge dx_2 \wedge dx_3,$$

so $C(x) = \vec{\nabla} \cdot \vec{B}$, and the exterior derivative on a 2-form gives the divergence of the corresponding vector.

$k = 3$**:** If C is a 3-form, dC is a 4-form. In three dimensions there cannot be any 4-forms, so $dC = 0$ for all such forms.

We can summarize the action of the exterior derivative in three dimensions in this diagram:

$$f \xrightarrow[\nabla f]{d} \omega^{(1)} \sim \vec{A} \xrightarrow[\nabla \times A]{d} \omega^{(2)} \sim \vec{B} \xrightarrow[\nabla \cdot B]{d} \omega^{(3)}$$

Now that we have d operating on all k-forms, we can ask what happens if we apply it twice. Looking first in three dimenions, on a 0-form we get $d^2 f = dA$ for $\vec{A} \sim \nabla f$, and $dA \sim \nabla \times A$, so $d^2 f \sim \nabla \times \nabla f$. But the curl of a gradient is zero, so $d^2 = 0$ in this case. On a one form $d^2 A = dB$, $\vec{B} \sim \nabla \times \vec{A}$ and $dB \sim \nabla \cdot B = \nabla \cdot (\nabla \times \vec{A})$. Now we have the divergence of a curl, which is also zero. For higher forms in three dimensions we can only get zero because the degree of the form would be greater than three. Thus we have a strong hint that d^2 might vanish in general. To verify this, we apply d^2 to $\omega^{(k)} = \sum \omega_{i_1 \ldots i_k} dx_{i_1} \wedge \cdots \wedge dx_{i_k}$. Then

$$\begin{aligned}
d\omega &= \sum_j \sum_{i_1<i_2<\cdots<i_k} \left(\partial_j \omega_{i_1 \ldots i_k}\right) dx_j \wedge dx_{i_1} \wedge \cdots \wedge dx_{i_k} \\
d(d\omega) &= \sum_{\ell j} \sum_{i_1<i_2<\cdots<i_k} \Big(\underbrace{\partial_\ell \partial_j}_{\text{symmetric}} \; \omega_{i_1 \ldots i_k} \Big) \underbrace{dx_\ell \wedge dx_j}_{\text{antisymmetric}} \wedge dx_{i_1} \wedge \cdots \wedge dx_{i_k} \\
&= 0.
\end{aligned}$$

This is a very important result. A k-form which is the exterior derivative of some $(k-1)$-form is called **exact**, while a k-form whose exterior

derivative vanishes is called **closed**, and we have just proven that all exact k-forms are closed.

The converse is a more subtle question. In general, there are k-forms which are closed but not exact, given by harmonic functions on the manifold $\mathcal{M}$, which form what is known as the cohomology of $\mathcal{M}$. This has to do with global properties of the space, however, and locally every closed form can be written as an exact one.[4] The precisely stated theorem, known as **Poincaré's Lemma**, is that if ω is a closed k-form on a coordinate neighborhood U of a manifold M, and if U is contractible to a point, then ω is exact on U. We will ignore the possibility of global obstructions and assume that we can write closed k-forms in terms of an exterior derivative acting on a $(k-1)$-form.

Coordinate independence of k-forms

We have introduced forms in a way which makes them appear dependent on the coordinates x_i used to describe the space $\mathcal{M}$. This is not what we want at all[5]. We want to be able to describe physical quantities that have intrinsic meaning independent of a coordinate system. If we are presented with another set of coordinates y_j describing the same physical space, the points in this space set up a mapping, ideally an isomorphism, from one coordinate space to the other, $\vec{y} = \vec{y}(\vec{x})$. If a function represents a physical field independent of coordinates, the actual function $f(x)$ used with the x coordinates must be replaced by

[4] An example may be useful. In two dimensions, the 1-form $\omega = -yr^{-2}dx + xr^{-2}dy$ satisfies $d\omega = 0$ wherever it is well defined, but it is not well defined at the origin. Locally, we can write $\omega = d\theta$, where θ is the polar coordinate. But θ is not, strictly speaking, a function on the plane, even on the plane with the origin removed, because it is not single-valued. It is a well defined function on the plane with a half axis removed, which leaves a simply-connected region, a region with no holes. In fact, this is the general condition for the exactness of a 1-form — a closed 1-form on a simply connected manifold is exact.

[5] Indeed, most mathematical texts will first define an abstract notion of a vector in the tangent space as a directional derivative operator, specified by equivalence classes of parameterized paths on $\mathcal{M}$. Then 1-forms are defined as duals to these vectors. In the first step any coordinatization of $\mathcal{M}$ is tied to the corresponding basis of the vector space $\mathbb{R}^n$. While this provides an elegant coordinate-independent way of defining the forms, the abstract nature of this definition of vectors can be unsettling to a physicist.

another function $\tilde{f}(y)$ when using the y coordinates. That they both describe the physical value at a given physical point requires $f(x) = \tilde{f}(y)$ when $y = y(x)$, or more precisely[6] $f(x) = \tilde{f}(y(x))$. This associated function and coordinate system is called a scalar field.

If we think of the differential df as the change in f corresponding to an infinitesimal change dx, then clearly $d\tilde{f}$ is the same thing in different coordinates, provided we understand the dy_i to represent the same physical displacement as dx does. That means

$$dy_k = \sum_j \frac{\partial y_k}{\partial x_j} dx_j.$$

As $f(x) = \tilde{f}(y(x))$ and $\tilde{f}(y) = f(x(y))$, the chain rule gives

$$\frac{\partial f}{\partial x_i} = \sum_j \frac{\partial \tilde{f}}{\partial y_j}\frac{\partial y_j}{\partial x_i}, \qquad \frac{\partial \tilde{f}}{\partial y_j} = \sum_i \frac{\partial f}{\partial x_i}\frac{\partial x_i}{\partial y_j},$$

so

$$\begin{aligned} d\tilde{f} &= \sum_k \frac{\partial \tilde{f}}{\partial y_k} dy_k = \sum_{ijk} \frac{\partial f}{\partial x_i}\frac{\partial x_i}{\partial y_k}\frac{\partial y_k}{\partial x_j} dx_j \\ &= \sum_{ij} \frac{\partial f}{\partial x_i}\delta_{ij} dx_j = \sum_i f_{,i} dx_i = df. \end{aligned}$$

We impose this transformation law in general on the coefficients in our k-forms, to make the k-form invariant, which means that the coefficients are covariant,

$$\begin{aligned} \tilde{\omega}_j &= \sum_i \frac{\partial x_i}{\partial y_j}\omega_i \\ \tilde{\omega}_{j_1 \ldots j_k} &= \sum_{i_1, i_2, \ldots, i_k} \left(\prod_{\ell=1}^{k} \frac{\partial x_{i_\ell}}{\partial y_{j_l}} \right) \omega_{i_1 \ldots i_k}. \end{aligned}$$

[6] More elegantly, giving the map $x \to y$ the name ϕ, so $y = \phi(x)$, we can state the relation as $f = \tilde{f} \circ \phi$.

Integration of k-forms

Suppose we have a k-dimensional smooth "surface" S in $\mathcal{M}$, parameterized by coordinates $(u_1, \cdots, u_k)$. We define the integral of a k-form

$$\omega^{(k)} = \sum_{i_1<\ldots<i_k} \omega_{i_1\ldots i_k} dx_{i_1} \wedge \cdots \wedge dx_{i_k}$$

over S by

$$\int_S \omega^{(k)} = \int \sum_{i_1,i_2,\ldots,i_k} \omega_{i_1\ldots i_k}(x(u)) \left(\prod_{\ell=1}^{k} \frac{\partial x_{i_\ell}}{\partial u_\ell} \right) du_1 du_2 \cdots du_k.$$

We had better give some examples. For $k = 1$, the "surface" is actually a path $\Gamma : u \mapsto x(u)$, and

$$\int_\Gamma \sum \omega_i dx_i = \int_{u_{\min}}^{u_{\max}} \sum \omega_i(x(u)) \frac{\partial x_i}{\partial u} du,$$

which seems obvious. In vector notation this is $\int_\Gamma \vec{A} \cdot d\vec{r}$, the path integral of the vector $\vec{A}$.

For $k = 2$,

$$\int_S \omega^{(2)} = \int B_{ij} \frac{\partial x_i}{\partial u} \frac{\partial x_j}{\partial v} du dv.$$

In three dimensions, the parallelogram which is the image of the rectangle $[u, u+du] \times [v, v+dv]$ has edges $(\partial\vec{x}/\partial u)du$ and $(\partial\vec{x}/\partial v)dv$, which has an area equal to the magnitude of

$$\text{“}d\vec{S}\text{”} = \left(\frac{\partial \vec{x}}{\partial u} \times \frac{\partial \vec{x}}{\partial v} \right) du dv$$

and a normal in the direction of “$d\vec{S}$”. Writing B_{ij} in terms of the corresponding vector $\vec{B}$, $B_{ij} = \epsilon_{ijk} B_k$, so

$$\begin{aligned} \int_S \omega^{(2)} &= \int_S \epsilon_{ijk} B_k \left(\frac{\partial \vec{x}}{\partial u} \right)_i \left(\frac{\partial \vec{x}}{\partial v} \right)_j du dv \\ &= \int_S B_k \left(\frac{\partial \vec{x}}{\partial u} \times \frac{\partial \vec{x}}{\partial v} \right)_k du dv = \int_S \vec{B} \cdot d\vec{S}, \end{aligned}$$

so $\int \omega^{(2)}$ gives the flux of $\vec{B}$ through the surface.

Similarly for $k = 3$ in three dimensions,

$$\sum \epsilon_{ijk} \left(\frac{\partial \vec{x}}{\partial u}\right)_i \left(\frac{\partial \vec{x}}{\partial v}\right)_j \left(\frac{\partial \vec{x}}{\partial w}\right)_k du dv dw$$

is the volume of the parallelopiped which is the image of $[u, u + du] \times [v, v + dv] \times [w, w + dw]$. As $\omega_{ijk} = \omega_{123}\epsilon_{ijk}$, this is exactly what appears:

$$\int \omega^{(3)} = \int \sum \epsilon_{ijk}\omega_{123} \frac{\partial x_i}{\partial u}\frac{\partial x_j}{\partial v}\frac{\partial x_k}{\partial w} du dv dw = \int \omega_{123}(x) dV.$$

Notice that we have only defined the integration of k-forms over submanifolds of dimension k, not over other-dimensional submanifolds. These are the only integrals which have coordinate invariant meanings.

We state[7] a marvelous theorem, special cases of which you have seen often before, known as **Stokes' Theorem**. Let C be a k-dimensional submanifold of $\mathcal{M}$, with ∂C its boundary. Let ω be a $(k-1)$-form. Then Stokes' theorem says

$$\int_C d\omega = \int_{\partial C} \omega. \tag{6.11}$$

This elegant jewel is actually familiar in several contexts in three dimensions. If $k = 2$, C is a surface, usually called S, bounded by a closed path $\Gamma = \partial S$. If ω is a 1-form associated with $\vec{A}$, then $\int_\Gamma \omega = \int_\Gamma \vec{A} \cdot d\vec{\ell}$. $d\omega$ is the 2-form $\sim \vec{\nabla} \times \vec{A}$, and $\int_S d\omega = \int_S \left(\vec{\nabla} \times \vec{A}\right) \cdot d\vec{S}$, so we see that this Stokes' theorem includes the one we first learned by that name. But it also includes other possibilities. We can try $k = 3$, where $C = V$ is a volume with surface $S = \partial V$. Then if $\omega \sim \vec{B}$ is a two form, $\int_S \omega = \int_S \vec{B} \cdot d\vec{S}$, while $d\omega \sim \vec{\nabla} \cdot \vec{B}$, so $\int_V d\omega = \int \vec{\nabla} \cdot \vec{B} dV$, so here Stokes' general theorem gives Gauss's theorem. Finally, we could consider $k = 1$, $C = \Gamma$, which has a boundary ∂C consisting of two points, say A and B. Our 0-form $\omega = f$ is a function, and Stokes' theorem gives[8] $\int_\Gamma f = f(B) - f(A)$, the "fundamental theorem of calculus".

[7] For a proof and for a more precise explanation of its meaning, we refer the reader to the mathematical literature. In particular [10] and [3] are advanced calculus texts which give elementary discussions in Euclidean 3-dimensional space. A more general treatment is (possibly???) given in [11].

[8] Note that there is a direction associated with the boundary, which is induced

6.6 The natural symplectic 2-form

We now turn our attention back to phase space, with a set of canonical coordinates (q_i, p_i). Using these coordinates we can define a particular 1-form $\omega_1 = \sum_i p_i dq_i$. For a point transformation $Q_i = Q_i(q_1, \ldots, q_n, t)$ we may use the same Lagrangian, reexpressed in the new variables, of course. Here the Q_i are independent of the velocities $\dot{q}_j$, so on phase space[9] $dQ_i = \sum_j (\partial Q_i/\partial q_j) dq_j$. The new velocities are given by

$$\dot{Q}_i = \sum_j \frac{\partial Q_i}{\partial q_j}\dot{q}_j + \frac{\partial Q_i}{\partial t}.$$

Thus the old canonical momenta,

$$p_i = \left.\frac{\partial L(q,\dot{q},t)}{\partial \dot{q}_i}\right|_{q,t} = \sum_j \left.\frac{\partial L(Q,\dot{Q},t)}{\partial \dot{Q}_j}\right|_{q,t} \left.\frac{\partial \dot{Q}_j}{\partial \dot{q}_i}\right|_{q,t} = \sum_j P_j \frac{\partial Q_j}{\partial q_i}.$$

Thus the form ω_1 may be written

$$\omega_1 = \sum_i \sum_j P_j \frac{\partial Q_j}{\partial q_i} dq_i = \sum_j P_j dQ_j,$$

so the form of ω_1 is invariant under point transformations. This is too limited, however, for our current goals of considering general canonical transformations on phase space, under which ω_1 will not be invariant. However, its exterior derivative

$$\omega_2 := d\omega_1 = \sum_i dp_i \wedge dq_i$$

is invariant under all canonical transformations, as we shall show momentarily. This makes it special, the **natural symplectic structure**

by a direction associated with C itself. This gives an ambiguity in what we have stated, for example how the direction of an open surface induces a direction on the closed loop which bounds it. Changing this direction would clearly reverse the sign of $\int \vec{A}\cdot d\vec{\ell}$. We have not worried about this ambiguity, but we cannot avoid noticing the appearence of the sign in this last example.

[9] We have not included a term $\frac{\partial Q_i}{\partial t} dt$ which would be necessary if we were considering a form in the $2n+1$ dimensional extended phase space which includes time as one of its coordinates.

on phase space. We can reexpress ω_2 in terms of our combined coordinate notation η_i, because

$$-\sum_{i<j} J_{ij} d\eta_i \wedge d\eta_j = -\sum_i dq_i \wedge dp_i = \sum_i dp_i \wedge dq_i = \omega_2.$$

We must now show that the natural symplectic structure is indeed form invariant under canonical transformation. Thus if Q_i, P_i are a new set of canonical coordinates, combined into ζ_j, we expect the corresponding object formed from them, $\omega_2' = -\sum_{ij} J_{ij} d\zeta_i \otimes d\zeta_j$, to reduce to the same 2-form, ω_2. We first note that

$$d\zeta_i = \sum_j \frac{\partial \zeta_i}{\partial \eta_j} d\eta_j = \sum_j M_{ij} d\eta_j,$$

with the same Jacobian matrix M we met in (6.3). Thus

$$\begin{aligned} \omega_2' &= -\sum_{ij} J_{ij} d\zeta_i \otimes d\zeta_j = -\sum_{ij} J_{ij} \sum_k M_{ik} d\eta_k \otimes \sum_\ell M_{j\ell} d\eta_\ell \\ &= -\sum_{k\ell} \left(M^T \cdot J \cdot M \right)_{k\ell} d\eta_k \otimes d\eta_\ell. \end{aligned}$$

Things will work out if we can show $M^T \cdot J \cdot M = J$, whereas what we know for canonical transformations from Eq. (6.3) is that $M \cdot J \cdot M^T = J$. We also know M is invertible and that $J^2 = -1$, so if we multiply this equation from the left by $-J \cdot M^{-1}$ and from the right by $J \cdot M$, we learn that

$$\begin{aligned} -J \cdot M^{-1} \cdot M \cdot J \cdot M^T \cdot J \cdot M &= -J \cdot M^{-1} \cdot J \cdot J \cdot M \\ &= J \cdot M^{-1} \cdot M = J \\ = -J \cdot J \cdot M^T \cdot J \cdot M &= M^T \cdot J \cdot M, \end{aligned}$$

which is what we wanted to prove. Thus we have shown that the 2-form ω_2 is form-invariant under canonical transformations, and deserves its name.

One important property of of the 2-form ω_2 on phase space is that it is **non-degenerate**; there is no vector $\vec{v}$ such that $\omega(\cdot, \vec{v}) = 0$, which follows simply from the fact that the matrix J_{ij} is non-singular.

Extended phase space

One way of looking at the evolution of a system is in phase space, where a given system corresponds to a point moving with time, and the general equations of motion corresponds to a velocity field. Another way is to consider **extended phase space**, a $2n+1$ dimensional space with coordinates (q_i, p_i, t), for which a system's motion is a path, monotone in t. By the modified Hamilton's principle, the path of a system in this space is an extremum of the action $I = \int_{t_i}^{t_f} \sum p_i dq_i - H(q,p,t)dt$, which is the integral of the one-form

$$\omega_3 = \sum p_i dq_i - H(q,p,t)dt.$$

The exterior derivative of this form involves the symplectic structure, ω_2, as $d\omega_3 = \omega_2 - dH \wedge dt$. The 2-form ω_2 on phase space is non-degenerate, and every vector in phase space is also in extended phase space. On such a vector, on which dt gives zero, the extra term gives only something in the dt direction, so there are still no vectors in this subspace which are annihilated by $d\omega_3$. Thus there is at most one direction in extended phase space which is annihilated by $d\omega_3$. But any 2-form in an odd number of dimensions must annihilate some vector, because in a given basis it corresponds to an antisymmetric matrix B_{ij}, and in an odd number of dimensions $\det B = \det B^T = \det(-B) = (-1)^{2n+1} \det B = -\det B$, so $\det B = 0$ and the matrix is singular, annihilating some vector ξ. In fact, for $d\omega_3$ this annihilated vector ξ is the tangent to the path the system takes through extended phase space.

One way to see this is to simply work out what $d\omega_3$ is and apply it to the vector ξ, which is proportional to $\vec{v} = (\dot{q}_i, \dot{p}_i, 1)$. So we wish to show $d\omega_3(\cdot, \vec{v}) = 0$. Evaluating

$$\begin{aligned}
\sum dp_i \wedge dq_i(\cdot, \vec{v}) &= \sum dp_i\, dq_i(\vec{v}) - \sum dq_i\, dp_i(\vec{v}) = \sum dp_i \dot{q}_i - \sum dq_i \dot{p}_i \\
dH \wedge dt(\cdot, \vec{v}) &= dH\, dt(\vec{v}) - dt\, dH(\vec{v}) \\
&= \left(\sum \frac{\partial H}{\partial q_i} dq_i + \sum \frac{\partial H}{\partial p_i} dp_i + \frac{\partial H}{\partial t} dt \right) 1 \\
&\quad -dt \left(\sum \dot{q}_i \frac{\partial H}{\partial q_i} + \sum \dot{p}_i \frac{\partial H}{\partial p_i} + \frac{\partial H}{\partial t} \right)
\end{aligned}$$

$$\begin{aligned} &= \sum \frac{\partial H}{\partial q_i} dq_i + \sum \frac{\partial H}{\partial p_i} dp_i - dt \sum \left(\dot{q}_i \frac{\partial H}{\partial q_i} + \dot{p}_i \frac{\partial H}{\partial p_i} \right) \\ d\omega_3(\cdot, \vec{v}) &= \sum \left(\dot{q}_i - \frac{\partial H}{\partial p_i} \right) dp_i - \left(\dot{p}_i + \frac{\partial H}{\partial q_i} \right) dq_i \\ &\quad + \sum \left(\dot{q}_i \frac{\partial H}{\partial q_i} + \dot{p}_i \frac{\partial H}{\partial p_i} \right) dt \\ &= 0 \end{aligned}$$

where the vanishing is due to the Hamilton equations of motion.

There is a more abstract way of understanding why $d\omega_3(\cdot, \vec{v})$ vanishes, from the modified Hamilton's principle, which states that if the path taken were infinitesimally varied from the physical path, there would be no change in the action. But this change is the integral of ω_3 along a loop, forwards in time along the first trajectory and backwards along the second. From Stokes' theorem this means the integral of $d\omega_3$ over a surface connecting these two paths vanishes. But this surface is a sum over infinitesimal parallelograms one side of which is $\vec{v}\,\Delta t$ and the other side of which[10] is $(\delta\vec{q}(t), \delta\vec{p}(t), 0)$. As this latter vector is an arbitrary function of t, each parallelogram must independently give 0, so that its contribution to the integral, $d\omega_3((\delta\vec{q}, \delta\vec{p}, 0), \vec{v})\Delta t = 0$. In addition, $d\omega_3(\vec{v}, \vec{v}) = 0$, of course, so $d\omega_3(\cdot, \vec{v})$ vanishes on a complete basis of vectors and is therefore zero.

6.6.1 Generating Functions

Consider a canonical transformation $(q, p) \to (Q, P)$, and the two 1-forms $\omega_1 = \sum_i p_i dq_i$ and $\omega_1' = \sum_i P_i dQ_i$. We have mentioned that the difference of these will not vanish in general, but the exterior derivative of this difference, $d(\omega_1 - \omega_1') = \omega_2 - \omega_2' = 0$, so $\omega_1 - \omega_1'$ is an closed 1-form. Thus it is exact[11], and there must be a function F on phase space such that $\omega_1 - \omega_1' = dF$. We call F the **generating function of the**

[10] It is slightly more elegant to consider the path parameterized independently of time, and consider arbitrary variations $(\delta q, \delta p, \delta t)$, because the integral involved in the action, being the integral of a 1-form, is independent of the parameterization. With this approach we find immediately that $d\omega_3(\cdot, \vec{v})$ vanishes on all vectors.

[11] We are assuming phase space is simply connected, or else we are ignoring any complications which might ensue from F not being globally well defined.

canonical transformation. If the transformation $(q,p) \to (Q,P)$ is such that the old q's alone, without information about the old p's, do not impose any restrictions on the new Q's, then the dq and dQ are independent, and we can use q and Q to parameterize phase space[12]. Then knowledge of the function $F(q,Q)$ determines the transformation, as

$$p_i = \left.\frac{\partial F}{\partial q_i}\right|_Q, \qquad -P_i = \left.\frac{\partial F}{\partial Q_i}\right|_q.$$

If the canonical transformation depends on time, the function F will also depend on time. Now if we consider the motion in extended phase space, we know the phase trajectory that the system takes through extended phase space is determined by Hamilton's equations, which could be written in any set of canonical coordinates, so in particular there is some Hamiltonian $K(Q,P,t)$ such that the tangent to the phase trajectory, $\vec{v}$, is annihilated by $d\omega_3'$, where $\omega_3' = \sum P_i dQ_i - K(Q,P,t)dt$. Now in general knowing that two 2-forms both annihilate the same vector would not be sufficient to identify them, but in this case we also know that restricting $d\omega_3$ and $d\omega_3'$ to their action on the $dt = 0$ subspace gives the same 2-form ω_2. That is to say, if $\vec{u}$ and $\vec{u}'$ are two vectors with time components zero, we know that $(d\omega_3 - d\omega_3')(\vec{u},\vec{u}') = 0$. Any vector can be expressed as a multiple of $\vec{v}$ and some vector $\vec{u}$ with time component zero, and as both $d\omega_3$ and $d\omega_3'$ annihilate $\vec{v}$, we see that $d\omega_3 - d\omega_3'$ vanishes on all pairs of vectors, and is therefore zero. Thus $\omega_3 - \omega_3'$ is a closed 1-form, which must be at least locally exact, and indeed $\omega_3 - \omega_3' = dF$, where F is the generating function we found above[13]. Thus $dF = \sum pdq - \sum PdQ + (K-H)dt$, or

$$K = H + \frac{\partial F}{\partial t}.$$

The function $F(q,Q,t)$ is what Goldstein calls F_1. The existence of F as a function on extended phase space holds even if the Q and q

[12]Note that this is the opposite extreme from a point transformation, which is a canonical transformation for which the Q's depend *only* on the q's, independent of the p's.

[13]From its definition in that context, we found that in phase space, $dF = \omega_1 - \omega_1'$, which is the part of $\omega_3 - \omega_3'$ not in the time direction. Thus if $\omega_3 - \omega_3' = dF'$ for some other function F', we know $dF' - dF = (K' - K)dt$ for some new Hamiltonian function $K'(Q,P,t)$, so this corresponds to an ambiguity in K.

are not independent, but in this case F will need to be expressed as a function of other coordinates. Suppose the new P's and the old q's are independent, so we can write $F(q, P, t)$. Then define $F_2 = \sum Q_i P_i + F$. Then

$$\begin{aligned} dF_2 &= \sum Q_i\, dP_i + \sum P_i\, dQ_i + \sum p_i\, dq_i - \sum P_i\, dQ_i + (K - H)dt \\ &= \sum Q_i\, dP_i + \sum p_i\, dq_i + (K - H)dt, \end{aligned}$$

so

$$Q_i = \frac{\partial F_2}{\partial P_i}, \qquad p_i = \frac{\partial F_2}{\partial q_i}, \qquad K(Q, P, t) = H(q, p, t) + \frac{\partial F_2}{\partial t}.$$

The generating function can be a function of old momenta rather than the old coordinates. Making one choice for the old coordinates and one for the new, there are four kinds of generating functions as described by Goldstein. Let us consider some examples. The function $F_1 = \sum_i q_i Q_i$ generates an interchange of p and q,

$$Q_i = p_i, \qquad P_i = -q_i,$$

which leaves the Hamiltonian unchanged. We saw this clearly leaves the form of Hamilton's equations unchanged. An interesting generator of the second type is $F_2 = \sum_i \lambda_i q_i P_i$, which gives $Q_i = \lambda_i q_i$, $P_i = \lambda_i^{-1} p_i$, a simple change in scale of the coordinates with a corresponding inverse scale change in momenta to allow $[Q_i, P_j] = \delta_{ij}$ to remain unchanged. This also doesn't change H. For $\lambda = 1$, this is the identity transformation, for which $F = 0$, of course.

Placing point transformations in this language provides another example. For a point transformation, $Q_i = f_i(q_1, \ldots, q_n, t)$, which is what one gets with a generating function

$$F_2 = \sum_i f_i(q_1, \ldots, q_n, t) P_i.$$

Note that

$$p_i = \frac{\partial F_2}{\partial q_i} = \sum_j \frac{\partial f_j}{\partial q_i} P_j$$

is at any point $\vec{q}$ a linear transformation of the momenta, required to preserve the canonical Poisson bracket, but this transformation is $\vec{q}$

dependent, so while $\vec{Q}$ is a function of $\vec{q}$ and t only, independent of $\vec{p}$, $\vec{P}(q,p,t)$ will in general have a nontrivial dependence on coordinates as well as a linear dependence on the old momenta.

For a harmonic oscillator, a simple scaling gives

$$H = \frac{p^2}{2m} + \frac{k}{2}q^2 = \frac{1}{2}\sqrt{k/m}\left(P^2 + Q^2\right),$$

where $Q = (km)^{1/4}q$, $P = (km)^{-1/4}p$. In this form, thinking of phase space as just some two-dimensional space, we seem to be encouraged to consider a new, polar, coordinate system with $\theta = \tan^{-1} Q/P$ as the new coordinate, and we might hope to have the radial coordinate related to the new momentum, $\mathcal{P} = -\partial F_1/\partial\theta$. As $P = \partial F_1/\partial Q$ is also $Q\cot\theta$, we can take $F_1 = \frac{1}{2}Q^2\cot\theta$, so $\mathcal{P} = -\frac{1}{2}Q^2(-\csc^2\theta) = \frac{1}{2}Q^2(1 + P^2/Q^2) = \frac{1}{2}(Q^2+P^2) = H/\omega$. Note as F_1 is not time dependent, $K = H$ and is independent of θ, which is therefore an ignorable coordinate, so its conjugate momentum $\mathcal{P}$ is conserved. Of course $\mathcal{P}$ differs from the conserved Hamiltonian H only by the factor $\omega = \sqrt{k/m}$, so this is not unexpected. With H now linear in the new momentum $\mathcal{P}$, the conjugate coordinate θ grows linearly with time at the fixed rate $\dot{\theta} = \partial H/\partial\mathcal{P} = \omega$.

Infinitesimal generators, redux

Let us return to the infinitesimal canonical transformation

$$\zeta_i = \eta_i + \epsilon g_i(\eta_j).$$

$M_{ij} = \partial\zeta_i/\partial\eta_j = \delta_{ij} + \epsilon\partial g_i/\partial\eta_j$ needs to be symplectic, and so $G_{ij} = \partial g_i/\partial\eta_j$ satisfies the appropriate condition for the generator of a symplectic matrix, $G\cdot J = -J\cdot G^T$. For the generator of the canonical transformation, we need a perturbation of the generator for the identity transformation, which can't be in F_1 form (as (q,Q) are not independent), but is easily done in F_2 form, $F_2(q,P) = \sum_i q_iP_i + \epsilon G(q,P,t)$, with $p_i = \partial F_2/\partial q_i = P_i + \epsilon\partial G/\partial q_i$, $Q_i = \partial F_2/\partial P_i = q_i + \epsilon\partial G/\partial P_i$, or

$$\zeta = \begin{pmatrix} Q_i \\ P_i \end{pmatrix} = \begin{pmatrix} q_i \\ p_i \end{pmatrix} + \epsilon \begin{pmatrix} 0 & \mathbb{1} \\ -\mathbb{1} & 0 \end{pmatrix} \begin{pmatrix} \partial G/\partial q_i \\ \partial G/\partial p_i \end{pmatrix} = \eta + \epsilon J\cdot\nabla G,$$

where we have ignored higher order terms in ϵ in inverting the $q \to Q$ relation and in replacing $\partial G/\partial Q_i$ with $\partial G/\partial q_i$.

The change due to the infinitesimal transformation may be written in terms of Poisson bracket with the coordinates themselves:

$$\delta\eta = \zeta - \eta = \epsilon J \cdot \nabla G = \epsilon[\eta, G].$$

In the case of an infinitesimal transformation due to time evolution, the small parameter can be taken to be Δt, and $\delta\eta = \Delta t\, \dot{\eta} = \Delta t[H, \eta]$, so we see that the Hamiltonian acts as the generator of time translations, in the sense that it maps the coordinate η of a system in phase space into the coordinates the system will have, due to its equations of motion, at a slightly later time.

This last example encourages us to find another interpretation of canonical transformations. Up to now we have viewed the transformation as a change of variables describing an unchanged physical situation, just as the passive view of a rotation is to view it as a change in the description of an unchanged physical point in terms of a rotated set of coordinates. But rotations are also used to describe changes in the physical situation with regards to a fixed coordinate system[14], and similarly in the case of motion through phase space, it is natural to think of the canonical transformation generated by the Hamiltonian as describing the actual motion of a system through phase space rather than as a change in coordinates. More generally, we may view a canonical transformation as a **diffeomorphism**[15] of phase space onto itself, $g : \mathcal{M} \to \mathcal{M}$ with $g(q, p) = (Q, P)$.

For an infinitesimal canonical transformation, this active interpretation gives us a small displacement $\delta\eta = \epsilon[\eta, G]$ for every point η in phase space, so we can view G and its associated infinitesimal canonical transformation as producing a flow on phase space. G also builds a finite transformation by repeated application, so that we get a sequence on canonical transformations g^λ parameterized by $\lambda = n\Delta\lambda$. This sequence maps an initial η_0 into a sequence of points $g^\lambda\eta_0$, each generated from the previous one by the infinitesimal transformation $\Delta\lambda G$, so $g^{\lambda+\Delta\lambda}\eta_0 - g^\lambda\eta_0 = \Delta\lambda[g^\lambda\eta_0, G]$. In the limit $\Delta\lambda \to 0$, with

[14] We leave to Mach and others the question of whether this distinction is real.

[15] An isomorphism $g : \mathcal{M} \to \mathcal{N}$ is a 1-1 map with an image including all of $\mathcal{N}$ (onto), which is therefore invertible to form $g^{-1} : \mathcal{N} \to \mathcal{M}$. A diffeomorphism is an isomorphism g for which both g and g^{-1} are differentiable.

n allowed to grow so that we consider a finite range of λ, we have a one (continuous) parameter family of transformations $g^\lambda : \mathcal{M} \to \mathcal{M}$, satisfying the differential equation

$$\frac{dg^\lambda(\eta)}{d\lambda} = \left[g^\lambda \eta, G\right].$$

This differential equation defines a phase flow on phase space. If G is not a function of λ, this has the form of a differential equation solved by an exponential,

$$g^\lambda(\eta) = e^{\lambda[\cdot, G]}\eta,$$

which means

$$g^\lambda(\eta) = \eta + \lambda[\eta, G] + \frac{1}{2}\lambda^2[[\eta, G], G] + ...$$

In the case that the generating function is the Hamiltonian, $G = H$, this phase flow gives the evolution through time, λ is t, and the velocity field on phase space is given by $[\eta, G]$. If the Hamiltonian is time independent, the velocity field is fixed, and the solution is formally an exponential.

Let me review changes due to a generating function. In the passive picture, we view η and $\zeta = \eta + \delta\eta$ as alternative coordinatizations of the same physical point in phase space. Let us call this point A when expressed in terms of the η coordinates and A' in terms of ζ. For an infinitesimal generator $F_2 = \sum_i q_i P_i + \epsilon G$, $\delta\eta = \epsilon J \nabla G = \epsilon[\eta, G]$. A physical scalar defined by a function $u(\eta)$ changes its functional form to $\tilde{u}$, but not its value at a given physical point, so $\tilde{u}(A') = u(A)$. For the Hamiltonian, there is a change in value as well, for $\tilde{H}$ or $\tilde{K}$ is not the same as H, even at the corresponding point,

$$\tilde{K}(A') = H(A) + \frac{\partial F_2}{\partial t} = H(A) + \epsilon\frac{\partial G}{\partial t}.$$

Now consider an active view. Here a canonical transformation is thought of as moving the point in phase space, and at the same time changing the functions $u \to \tilde{u}$, $H \to \tilde{K}$, where we are focusing on the form of these functions, on how they depend on their arguments. We

think of ζ as representing a different point B of phase space, although the coordinates $\eta(B)$ are the same as $\zeta(A')$. We ask how $\tilde{u}$ and K differ from u and H at B. At the cost of differing from Goldstein by an overall sign, let

$$\begin{aligned}\Delta u &= \tilde{u}(B) - u(B) = u(A) - u(A') = -\delta\eta_i \frac{\partial u}{\partial \eta_i} = -\epsilon \sum_i [\eta_i, G] \frac{\partial u}{\partial \eta_i} \\ &= -\epsilon [u, G]\end{aligned}$$

$$\begin{aligned}\Delta H &= K(B) - H(B) = H(A) + \epsilon \frac{\partial G}{\partial t} - H(A') = \epsilon \left(\frac{\partial G}{\partial t} - [H, G] \right) \\ &= \epsilon \frac{dG}{dt}.\end{aligned}$$

Note that if the generator of the transformation is a conserved quantity, the Hamiltonian is unchanged, in that it is the same function after the transformation as it was before. That is, the Hamiltonian is **form invariant**.

We have seen that conserved quantities are generators of symmetries of the problem, transformations which can be made without changing the Hamiltonian. We saw that the symmetry generators form a closed algebra under Poisson bracket, and that finite symmetry transformations result from exponentiating the generators. Let us discuss the more common conserved quantities in detail, showing how they generate symmetries. We have already seen that ignorable coordinates lead to conservation of the corresponding momentum. Now the reverse comes if we assume one of the momenta, say p_I, is conserved. Then from our discussion we know that the generator $G = p_I$ will generate canonical transformations which are symmetries of the system. Those transformations are

$$\delta q_j = \epsilon [q_j, p_I] = \epsilon \delta_{jI}, \qquad \delta p_j = \epsilon [p_j, p_I] = 0.$$

Thus the transformation just changes the one coordinate q_I and leaves all the other coordinates and all momenta unchanged. In other words, it is a translation of q_I. As the Hamiltonian is unchanged, it must be independent of q_I, and q_I is an ignorable coordinate.

Second, consider the angular momentum component $\vec{\omega}\cdot\vec{L} = \epsilon_{ijk}\omega_i r_j p_k$ for a point particle with $q = \vec{r}$. As a generator, $\epsilon\vec{\omega}\cdot\vec{L}$ produces changes

$$\begin{aligned}\delta r_\ell &= \epsilon[r_\ell, \epsilon_{ijk}\omega_i r_j p_k] = \epsilon\epsilon_{ijk}\omega_i r_j [r_\ell, p_k] = \epsilon\epsilon_{ijk}\omega_i r_j \delta_{\ell k} = \epsilon\epsilon_{ij\ell}\omega_i r_j \\ &= \epsilon(\vec{\omega}\times\vec{r})_\ell,\end{aligned}$$

which is how the point moves under a rotation about the axis $\vec{\omega}$. The momentum also changes,

$$\begin{aligned}\delta p_\ell &= \epsilon[p_\ell, \epsilon_{ijk}\omega_i r_j p_k] = \epsilon\epsilon_{ijk}\omega_i p_k [p_\ell, r_j] = \epsilon\epsilon_{ijk}\omega_i p_k(-\delta_{\ell j}) = -\epsilon\epsilon_{i\ell k}\omega_i p_k \\ &= \epsilon(\vec{\omega}\times\vec{p})_\ell,\end{aligned}$$

so $\vec{p}$ also rotates.

By Poisson's theorem, the set of constants of the motion is closed under Poisson bracket, and given two such generators, the bracket is also a symmetry, so the symmetries form a Lie algebra under Poisson bracket. For a free particle, $\vec{p}$ and $\vec{L}$ are both symmetries, and we have just seen that $[p_\ell, L_i] = \epsilon_{ik\ell}p_k$, a linear combination of symmetries, while of course $[p_i, p_j] = 0$ generates the identity transformation and is in the algebra. What about $[L_i, L_j]$? As $L_i = \epsilon_{ik\ell}r_k p_\ell$,

$$\begin{aligned}[L_i, L_j] &= [\epsilon_{ik\ell}r_k p_\ell, L_j] \\ &= \epsilon_{ik\ell}r_k[p_\ell, L_j] + \epsilon_{ik\ell}[r_k, L_j]p_\ell \\ &= -\epsilon_{ik\ell}r_k\epsilon_{j\ell m}p_m + \epsilon_{ik\ell}\epsilon_{jmk}r_m p_\ell \\ &= (\delta_{ij}\delta_{km} - \delta_{im}\delta_{jk})\, r_k p_m - (\delta_{ij}\delta_{m\ell} - \delta_{im}\delta_{j\ell})\, r_m p_\ell \\ &= (\delta_{ia}\delta_{jb} - \delta_{ib}\delta_{ja})\, r_a p_b \\ &= \epsilon_{kij}\epsilon_{kab}r_a p_b = \epsilon_{ijk}L_k. \qquad (6.12)\end{aligned}$$

We see that we get back the third component of $\vec{L}$, so we do not get a new kind of conserved quantity, but instead we see that the algebra closes on the space spanned by the momenta and angular momenta. We also note that it is impossible to have two components of $\vec{L}$ conserved without the third component also being conserved. Note also that $\vec{\omega}\cdot\vec{L}$ does a rotation the same way on the three vectors $\vec{r}$, $\vec{p}$, and $\vec{L}$. Indeed it will do so on any vector composed from $\vec{r}$, and $\vec{p}$, rotating all of the physical system[16].

[16]If there is some rotationally non-invariant property of a particle which is not

The above algebraic artifice is peculiar to three dimensions; in other dimensions $d \neq 3$ there is no ϵ-symbol to make a vector out of L, but the angular momentum can always be treated as an antisymmetric tensor, $L_{ij} = x_i p_j - x_j p_i$. There are $D(D-1)/2$ components, and the Lie algebra again closes

$$[L_{ij}, L_{k\ell}] = \delta_{jk} L_{i\ell} - \delta_{ik} L_{j\ell} - \delta_{j\ell} L_{ik} + \delta_{i\ell} L_{jk}.$$

We have related conserved quantities to generators of infinitesimal canonical transformation, but these infinitesimals can be integrated to produce finite transformations as well. Suppose we consider a parameterized set of canonical transformations $\eta \to \zeta(\alpha)$, as a sequence of transformations generated by $\delta\alpha\, G$ acting repeatedly, so that

$$\begin{aligned} \zeta(\alpha + \delta\alpha) &= \zeta(\alpha) + \delta\alpha [\zeta(\alpha), G] \\ \text{or } \frac{d\zeta}{d\alpha} &= [\zeta, G]. \end{aligned}$$

The right side is linear in ζ, so the solution of this differential equation is, at least formally,

$$\begin{aligned} \zeta(\alpha) &= e^{[\cdot, G]} \zeta(0) \\ &= \left(1 + \alpha[\cdot, G] + \frac{1}{2}\alpha^2 [[\cdot, G], G] + ...\right) \zeta(0) \\ &= \zeta(0) + \alpha[\zeta(0), G] + \frac{1}{2}\alpha^2 [[\zeta(0), G], G] + ... \end{aligned}$$

In this fashion, any Lie algebra, and in particular the Lie algebra formed by the Poisson brackets of generators of symmetry transformations, can be exponentiated to form a continuous group, called a Lie Group. In the case of angular momentum, the three components form a three-dimensional Lie algebra, and the exponentials of these a three-dimensional Lie group which is $SO(3)$, the rotation group.

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built out of $\vec{r}$ and $\vec{p}$, it will not be suitably rotated by $\vec{L} = \vec{r} \times \vec{p}$, in which case $\vec{L}$ is not the full angular momentum but only the **orbital angular momentum**. The generator of a rotation of all of the physics, the full angular momentum $\vec{J}$, is then the sum of $\vec{L}$ and another piece, called the **intrinsic spin** of the particle.

6.7 Hamilton–Jacobi Theory

We have mentioned the time dependent canonical transformation that maps the coordinates of a system at a given fixed time t_0 into their values at a later time t. Now let us consider the reverse transformation, mapping $(q(t), p(t)) \to (Q = q_0, P = p_0)$. But then $\dot{Q} = 0$, $\dot{P} = 0$, and the Hamiltonian which generates these trivial equations of motion is $K = 0$. We denote by $S(q, P, t)$ the generating function of type 2 which generates this transformation. It satisfies

$$K = H(q, p, t) + \frac{\partial S}{\partial t} = 0, \qquad \text{with } p_i = \frac{\partial S}{\partial q_i},$$

so S is determined by the differential equation

$$H\left(q, \frac{\partial S}{\partial q}, t\right) + \frac{\partial S}{\partial t} = 0, \tag{6.13}$$

which we can think of as a partial differential equation in $n+1$ variables q, t, thinking of P as fixed and understood. If H is independent of time, we can solve by separating the t from the q dependence, we may write $S(q, P, t) = W(q, P) - \alpha t$, where α is the separation constant independent of q and t, but not necessarily of P. We get a time-independent equation

$$H\left(q, \frac{\partial W}{\partial q}\right) = \alpha. \tag{6.14}$$

The function S is known as **Hamilton's principal function**, while the function W is called **Hamilton's characteristic function**, and the equations (6.13) and (6.14) are both known as the **Hamilton-Jacobi** equation. They are still partial differential equations in many variables, but under some circumstances further separation of variables may be possible. We consider first a system with one degree of freedom, with a conserved H, which we will sometimes specify even further to the particular case of a harmonic oscillator. Then we we treat a separable system with two degrees of freedom.

We are looking for new coordinates (Q, P) which are time independent, and have the differential equation for Hamilton's principal

function $S(q, P, t)$:

$$H\left(q, \frac{\partial S}{\partial q}\right) + \frac{\partial S}{\partial t} = 0.$$

For a harmonic oscillator with $H = p^2/2m + \frac{1}{2}kq^2$, this equation is

$$\left(\frac{\partial S}{\partial q}\right)^2 + kmq^2 + 2m\frac{\partial S}{\partial t} = 0. \tag{6.15}$$

We can certainly find a seperated solution of the form $S = W(q, P) - \alpha(P)t$, where the first two terms of (6.15) are independent of t. Then we have an ordinary differential equation,

$$\left(\frac{dW}{dq}\right)^2 = 2m\alpha - kmq^2,$$

which can be easily integrated

$$\begin{aligned} W &= \int_0^q \sqrt{2m\alpha - kmq^2}\, dq + f(\alpha) \\ &= f(\alpha) + \frac{\alpha}{\omega}\left(\theta + \frac{1}{2}\sin 2\theta\right), \end{aligned} \tag{6.16}$$

where we have made a substitution $\sin\theta = q\sqrt{k/2\alpha}$, and made explicit note that the constant (in q) of integration, $f(\alpha)$, may depend on α. For other hamiltonians, we will still have the solution to the partial differential equation for S given by separation of variables $S = W(q, P) - \alpha t$, because H was assumed time-independent, but the integral for W may not be doable analytically.

As S is a type 2 generating function,

$$p = \frac{\partial F_2}{\partial q} = \frac{\partial W}{\partial q}.$$

For our harmonic oscillator, this gives

$$p = \frac{\partial W}{\partial \theta} \Big/ \frac{\partial q}{\partial \theta} = \frac{\alpha}{\omega}\frac{1 + \cos 2\theta}{\sqrt{2\alpha/k}\,\cos\theta} = \sqrt{2\alpha m}\cos\theta.$$

Plugging into the Hamiltonian, we have

$$H = \alpha(\cos^2\theta + \sin^2\theta) = \alpha,$$

which will always be the case when (6.14) holds.

We have not spelled out what our new momentum P is, except that it is conserved, and we can take it to be α. ($\alpha = \omega R$ in terms of our previous discussion of the harmonic oscillator.) The new coordinate $Q = \partial S/\partial P = \partial W/\partial\alpha|_q - t$. But Q is, by hypothesis, time independent, so

$$\frac{\partial W}{\partial \alpha} = t + Q.$$

For the harmonic oscillator calculation (6.16),

$$f'(\alpha) + \frac{1}{\omega}(\theta + \frac{1}{2}\sin 2\theta) + \frac{\alpha}{\omega}\left.\frac{\partial\theta}{\partial\alpha}\right|_q (1 + \cos 2\theta) = f'(\alpha) + \frac{\theta}{\omega} = t + Q$$

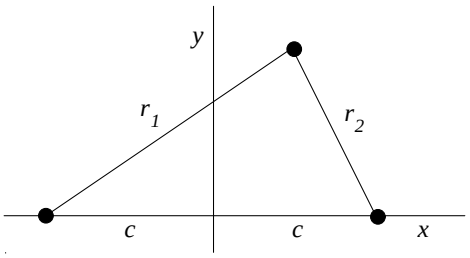
Recall $\sin\theta = q\sqrt{k/2\alpha}$, so

$$\left.\frac{\partial\theta}{\partial\alpha}\right|_q = \frac{-q}{2\alpha\cos\theta}\sqrt{\frac{k}{2\alpha}} = -\frac{1}{2\alpha}\tan\theta,$$

and $\theta = \omega t + \delta$, for δ some constant.

As an example of a nontrivial problem with two degrees of freedom which is nonetheless separable and therefore solvable using the Hamilton-Jacobi method, we consider the motion of a particle of mass m attracted by Newtonian gravity to two equal masses fixed in space. For simplicity we consider only motion in a plane containing the two masses, which we take to be at $(\pm c, 0)$ in cartesian coordinates x, y. If r_1 and r_2 are the distances from the particle to the two fixed masses respectively, the gravitational potential is $U = -K(r_1^{-1} + r_2^{-1})$, while the kinetic energy is simple in terms of x and y, $T = \frac{1}{2}m(\dot{x}^2 + \dot{y}^2)$. The relation between these is, of course,

$$\begin{aligned} r_1^2 &= (x+c)^2 + y^2 \\ r_2^2 &= (x-c)^2 + y^2 \end{aligned}$$



Considering both the kinetic and potential energies, the problem will not separate either in terms of (x, y) or in terms of (r_1, r_2), but it does separate in terms of elliptical coordinates

$$\begin{aligned} \xi &= r_1 + r_2 \\ \eta &= r_1 - r_2 \end{aligned}$$

From $r_1^2 - r_2^2 = 4cx = \xi\eta$ we find a fairly simple expression $\dot{x} = (\xi\dot{\eta} + \dot{\xi}\eta)/4c$. The expression for y is more difficult, but can be found from observing that $\frac{1}{2}(r_1^2 + r_2^2) = x^2 + y^2 + c^2 = (\xi^2 + \eta^2)/4$, so

$$y^2 = \frac{\xi^2 + \eta^2}{4} - \left(\frac{\xi\eta}{4c}\right)^2 - c^2 = \frac{(\xi^2 - 4c^2)(4c^2 - \eta^2)}{16c^2},$$

or

$$y = \frac{1}{4c}\sqrt{\xi^2 - 4c^2}\sqrt{4c^2 - \eta^2}$$

and

$$\dot{y} = \frac{1}{4c}\left(\xi\dot{\xi}\sqrt{\frac{4c^2 - \eta^2}{\xi^2 - 4c^2}} - \eta\dot{\eta}\sqrt{\frac{\xi^2 - 4c^2}{4c^2 - \eta^2}}\right).$$

Squaring, adding in the x contribution, and simplifying then shows that

$$T = \frac{m}{8}\left(\frac{\xi^2 - \eta^2}{4c^2 - \eta^2}\dot{\eta}^2 + \frac{\xi^2 - \eta^2}{\xi^2 - 4c^2}\dot{\xi}^2\right).$$

Note that there are no crossed terms $\propto \dot{\xi}\dot{\eta}$, a manifestation of the orthogonality of the curvilinear coordinates ξ and η. The potential energy becomes

$$U = -K\left(\frac{1}{r_1} + \frac{1}{r_2}\right) = -K\left(\frac{2}{\xi + \eta} + \frac{2}{\xi - \eta}\right) = \frac{-4K\xi}{\xi^2 - \eta^2}.$$

In terms of the new coordinates ξ and η and their conjugate momenta, we see that

$$H = \frac{2/m}{\xi^2 - \eta^2}\left(p_\xi^2(\xi^2 - 4c^2) + p_\eta^2(4c^2 - \eta^2) - 2mK\xi\right).$$

Then the Hamilton-Jacobi equation for Hamilton's characteristic function is

$$\frac{2/m}{\xi^2 - \eta^2}\left((\xi^2 - 4c^2)\left(\frac{\partial W}{\partial \xi}\right)^2 + (4c^2 - \eta^2)\left(\frac{\partial W}{\partial \eta}\right)^2 - 2mK\xi\right) = \alpha,$$

or

$$\begin{aligned}(\xi^2 - 4c^2)\left(\frac{\partial W}{\partial \xi}\right)^2 - 2mK\xi - \frac{1}{2}m\alpha\xi^2 \\ +(4c^2 - \eta^2)\left(\frac{\partial W}{\partial \eta}\right)^2 + \frac{1}{2}\alpha m\eta^2 = 0.\end{aligned}$$

The first line depends only on ξ, and the second only on η, so they must each be constant, with $W(\xi, \eta) = W_\xi(\xi) + W_\eta(\eta)$, and

$$\begin{aligned}(\xi^2 - 4c^2)\left(\frac{dW_\xi(\xi)}{d\xi}\right)^2 - 2mK\xi - \frac{1}{2}\alpha m\xi^2 &= \beta \\ (4c^2 - \eta^2)\left(\frac{dW_\eta(\eta)}{d\eta}\right)^2 + \frac{1}{2}\alpha m\eta^2 &= -\beta.\end{aligned}$$

These are now reduced to integrals for W_i, which can in fact be integrated to give an explicit expression in terms of elliptic integrals.

6.8 Action-Angle Variables

Consider again a general system with one degree of freedom and a conserved Hamiltonian. Suppose the system undergoes periodic behavior, with $p(t)$ and $\dot{q}(t)$ periodic with period τ. We don't require q itself to be periodic as it might be an angular variable which might not return to the same value when the system returns to the same physical point, as, for example, the angle which describes a rotation.

If we define an integral over one full period,

$$J(t) = \frac{1}{2\pi}\int_t^{t+\tau} p\,dq,$$

it will be time independent. As $p = \partial W/\partial q = p(q,\alpha)$, the integral can be defined without reference to time, just as the integral $2\pi J = \int p dq$ over one orbit of q, holding α fixed. Then J becomes a function of α alone, and if we assume this function to be invertible, $H = \alpha = \alpha(J)$. We can take J to be our canonical momentum P. Using Hamilton's Principal Function S as the generator, we find $Q = \partial S/\partial J = \partial W(q,J)/\partial J - (d\alpha/dJ)t$. Alternatively, we might use Hamilton's Characteristic Function W by itself as the generator, to define the conjugate variable $\phi = \partial W(q,J)/\partial J$, which is simply related to $Q = \phi - (d\alpha/dJ)t$. Note that ϕ and Q are both canonically conjugate to J, differing at any instant only by a function of J. As the Hamilton-Jacobi Q is time independent, we see that $\dot{\phi} = d\alpha/dJ = dH/dJ = \omega(J)$, which is a constant, because while it is a function of J, J is a constant in time. We could also derive $\dot{\phi}$ from Hamilton's equations considering W as a genenerator, for W is time independent, the therefore the new Hamiltonian is unchanged, and the equation of motion for ϕ is simply $\dot{\phi} = \partial H/\partial J$. Either way, we see that $\phi = \omega t + \delta$. The coordinates (J,ϕ) are called **action-angle** variables. Consider the change in ϕ during one cycle.

$$\Delta\phi = \oint \frac{\partial\phi}{\partial q}\,dq = \oint \left(\frac{\partial}{\partial q}\frac{\partial W}{\partial J}\right) dq = \frac{d}{dJ}\oint p dq = \frac{d}{dJ}2\pi J = 2\pi.$$

Thus we see that in one period τ, $\Delta\phi = 2\pi = \omega\tau$, so $\omega = 1/\tau$.

For our harmonic oscillator, of course,

$$2\pi J = \oint p dq = \sqrt{2\alpha m}\sqrt{\frac{2\alpha}{k}}\int_0^{2\pi}\cos^2\theta d\theta = \frac{2\alpha\pi}{\sqrt{k/m}}$$

so J is just a constant $1/\sqrt{k/m}$ times the old canonical momentum α, and thus its conjugate $\phi = \sqrt{k/m}\ Q = \sqrt{k/m}(t+\beta)$, so $\omega = \sqrt{k/m}$ as we expect. The important thing here is that $\Delta\phi = 2\pi$, even if the problem itself is not solvable.

Exercises

6.1 In Exercise 2.6, we discussed the connection between two Lagrangians, L_1 and L_2, which differed by a total time derivative of a function on extended configuration space,

$$L_1(\{q_i\},\{\dot{q}_j\},t) = L_2(\{q_i\},\{\dot{q}_j\},t) + \frac{d}{dt}\Phi(q_1,...,q_n,t).$$

You found that these gave the same equations of motion, but differing momenta $p_i^{(1)}$ and $p_i^{(2)}$. Find the relationship between the two Hamiltonians, H_1 and H_2, and show that these lead to equivalent equations of motion.

6.2 A uniform static magnetic field can be described by a static vector potential $\vec{A} = \frac{1}{2}\vec{B}\times\vec{r}$. A particle of mass m and charge q moves under the influence of this field.
(a) Find the Hamiltonian, using inertial cartesian coordinates.
(b) Find the Hamiltonian, using coordinates of a rotating system with angular velocity $\vec{\omega} = -q\vec{B}/2mc$.

6.3 Consider a symmetric top with one pont on the symmetry axis fixed in space, as we did at the end of chapter 4. Write the Hamiltonian for the top. Noting the cyclic (ignorable) coordinates, explain how this becomes an effective one-dimensional system.

6.4 (a) Show that a particle under a central force with an attractive *potential* inversely proportional to the distance *squared* has a conserved quantity $D = \frac{1}{2}\vec{r}\cdot\vec{p} - Ht$.
(b) Show that the infinitesimal transformation generated by D scales $\vec{r}$ and $\vec{p}$ by opposite infinitesimal amounts, $\vec{Q} = (1+\frac{\epsilon}{2})\vec{r}$, $\vec{P} = (1-\frac{\epsilon}{2})\vec{p}$, or for a finite transformation $\vec{Q} = \lambda\vec{r}$, $\vec{P} = \lambda^{-1}\vec{p}$. Show that if we describe the motion in terms of a scaled time $T = \lambda^2 t$, the equations of motion are invariant under this combined transformation $(\vec{r},\vec{p},t) \to (\vec{Q},\vec{P},T)$.

6.5 We saw that the Poisson bracket associates with every differentiable function f on phase space a differential operator $D_f := [f,\cdot]$ which acts on functions g on phase space by $D_f g = [f,g]$. We also saw that every differential operator is associated with a vector, which in a particular coordinate system has components f_i, where

$$D_f = \sum f_i \frac{\partial}{\partial\eta_i}.$$

A 1-form acts on such a vector by

$$dx_j(D_f) = f_j.$$

Show that for the natural symplectic structure ω_2, acting on the differential operator coming from the Poisson bracket as its first argument,

$$\omega_2(D_f, \cdot) = df,$$

which indicates the connection between ω_2 and the Poisson bracket.

6.6 Give a complete discussion of the relation of forms in cartesian coordinates in four dimensions to functions, vector fields, and antisymmetric matrix (tensor) fields, and what wedge products and exterior derivatives of the forms correspond to in each case. This discussion should parallel what is done in my book, Pages 148-150, for three dimensions. [Note that two different antisymmetric tensors, $B_{\mu\nu}$ and $\tilde{B}_{\mu\nu} = \frac{1}{2}\sum_{\rho\sigma}\epsilon_{\mu\nu\rho\sigma}B_{\rho\sigma}$, can be related to the same 2-form, in differing fashions. They are related to each other with the four dimensional $\epsilon_{jk\ell m}$, which you will need to define, and are called **duals** of each other. Using one fashion, the two different 2-forms associated with these two matrices are also called duals.
(b) Let $F_{\mu\nu}$ be a 4×4 matrix defined over a four dimensional space (x, y, z, ict), with matrix elements $F_{jk} = \epsilon_{jk\ell}B_\ell$, for j, k, ℓ each $1, 2, 3$, and $F_{4j} = iE_j = -F_{j4}$. Show that the statement that F corresponds, by one of the two fashions, to a closed 2-form F, constitutes two of Maxwell's equations, and explain how this implies that 2-form is the exterior derivative of a 1-form, and what that 1-form is in terms of electromagnetic theory described in 3-dimensional language.
(c) Find the 3-form associated with the exterior derivative of the 2-form dual to F, and show that it is associated with the 4-vector charge current density $J = (\vec{j}, ic\rho)$, where $\vec{j}$ is the usual current density and ρ the usual charge density.

6.7 Consider the following differential forms:

$$\begin{aligned}
A &= y\,dx + x\,dy + dz \\
B &= y^2\,dx + x^2\,dy + dz \\
C &= xy(y-x)\,dx \wedge dy + y(y-1)\,dx \wedge dz + x(x-1)\;dy \wedge dz \\
D &= 2(x-y)\,dx \wedge dy \wedge dz \\
E &= 2(x-y)\,dx \wedge dy
\end{aligned}$$

Find as many relations as you can, expressible without coordinates, among these forms. Consider using the exterior derivative and the wedge product.

Chapter 7

Perturbation Theory

The class of problems in classical mechanics which are amenable to exact solution is quite limited, but many interesting physical problems differ from such a solvable problem by corrections which may be considered small. One example is planetary motion, which can be treated as a perturbation on a problem in which the planets do not interact with each other, and the forces with the Sun are purely Newtonian forces between point particles. Another example occurs if we wish to find the first corrections to the linear small oscillation approximation to motion about a stable equilibrium point. The best starting point is an **integrable system**, for which we can find sufficient integrals of the motion to give the problem a simple solution in terms of action-angle variables as the canonical coordinates on phase space. One then phrases the full problem in such a way that the perturbations due to the extra interactions beyond the integrable forces are kept as small as possible. We first examine the solvable starting point.

7.1 Integrable systems

An integral of the motion for a hamiltonian system is a function F on phase space $\mathcal{M}$ for which the Poisson bracket with H vanishes, $[F, H] = 0$. More generally, a set of functions on phase space is said to be in **involution** if all their pairwise Poisson brackets vanish. The systems we shall consider are **integrable systems** in the sense that

there exists one integral of the motion for each degree of freedom, and these are in involution and independent. Thus on the $2n$-dimensional manifold of phase space, there are n functions F_i for which $[F_i, F_j] = 0$, and the F_i are independent, so the dF_i are linearly independent at each point $\eta \in \mathcal{M}$. We will assume the first of these is the Hamiltonian. As each of the F_i is a conserved quantity, the motion of the system is confined to a submanifold of phase space determined by the initial values of thes invariants $f_i = F_i(q(0), p(0))$:

$$\mathcal{M}_{\vec{f}} = \{\eta : F_i(\eta) = f_i \text{ for } i = 1, \ldots, n\}.$$

The differential operators $D_{F_i} = [F_i, \cdot]$ correspond to vectors tangent to the manifold $\mathcal{M}_{\vec{f}}$, because acting on each of the F_j functions D_{F_i} vanishes, as the F's are in involution. These differential operators also commute with one another, because as we saw in (6.9),

$$D_{F_i} D_{F_j} - D_{F_j} D_{F_i} = D_{[F_i, F_j]} = 0.$$

They are also linearly independent, for if $\sum \alpha_i D_{F_i} = 0$, $\sum \alpha_i D_{F_i} \eta_j = 0 = [\sum \alpha_i F_i, \eta_j]$, which means that $\sum \alpha_i F_i$ is a constant on phase space, and that would contradict the assumed independence of the F_i. Thus the D_{F_i} are n commuting independent differential operators corresponding to the generators F_i of an Abelian group of displacements on $\mathcal{M}_{\vec{f}}$. A given reference point $\eta_0 \in \mathcal{M}$ is mapped by the canonical transformation generator $\sum t_i F_i$ into some other point $g^{\vec{t}}(\eta_0) \in \mathcal{M}_{\vec{f}}$. If the manifold $\mathcal{M}_{\vec{f}}$ is compact, there must be many values of $\vec{t}$ for which $g^{\vec{t}}(\eta_0) = \eta_0$. These elements form an abelian subgroup, and therefore a lattice in $\mathbb{R}^n$. It has n independent lattice vectors, and a unit cell which is in 1-1 correspondence with $\mathcal{M}_{\vec{f}}$. Let these basis vectors be $\vec{e}_1, \ldots, \vec{e}_n$. These are the edges of the unit cell in $\mathbb{R}^n$, the interior of which is a linear combination $\sum a_i \vec{e}_i$ where each of the $a_i \in [0, 1)$. We therefore have a diffeomorphism between this unit cell and $\mathcal{M}_{\vec{f}}$, which induces coordinates on $\mathcal{M}_{\vec{f}}$. Because these are periodic, we scale the a_i to new coordinates $\phi_i = 2\pi a_i$, so each point of $\mathcal{M}_{\vec{f}}$ is labelled by $\vec{\phi}$, given by the $\vec{t} = \sum \phi_k \vec{e}_k / 2\pi$ for which $g^{\vec{t}}(\eta_0) = \eta$. Notice each ϕ_i is a coordinate on a circle, with $\phi_i = 0$ representing the same point as $\phi_i = 2\pi$, so the manifold $\mathcal{M}_{\vec{f}}$ is diffeomorphic to an n dimensional torus $T^n = (S^1)^n$.

Under an infinitesimal generator $\sum \delta t_i F_i$, a point of $\mathcal{M}_{\vec{f}}$ is translated by $\delta\eta = \sum \delta t_i [\eta, F_i]$. This is true for any choice of the coordinates η, in particular it can be applied to the ϕ_j, so

$$\delta\phi_j = \sum_i \delta t_i [\phi_j, F_i],$$

where we have already expressed

$$\delta\vec{t} = \sum_k \delta\phi_k \vec{e}_k / 2\pi.$$

We see that the Poisson bracket is the inverse of the matrix A_{ji} given by the j'th coordinate of the i'th basis vector

$$A_{ji} = \frac{1}{2\pi} (\vec{e}_i)_j , \qquad \delta\vec{t} = A \cdot \delta\phi, \qquad [\phi_j, F_i] = \left(A^{-1}\right)_{ji}.$$

As the Hamiltonian $H = F_1$ corresponds to the generator with $\vec{t} = (1, 0, \ldots, 0)$, an infinitesimal time translation generated by $\delta t H$ produces a change $\delta\phi_i = (A^{-1})_{i1}\delta t = \omega_i \delta t$, for some vector $\vec{\omega}$ which is determined by the $\vec{e}_i$. Note that the periodicities $\vec{e}_i$ may depend on the values of the integrals of the motion, so $\vec{\omega}$ does as well, and we have

$$\frac{d\vec{\phi}}{dt} = \vec{\omega}(\vec{f}).$$

The angle variables $\vec{\phi}$ are not conjugate to the integrals of the motion F_i, but rather to combinations of them,

$$I_i = \frac{1}{2\pi} \vec{e}_i(\vec{f}) \cdot \vec{F},$$

for then

$$[\phi_j, I_i] = \frac{1}{2\pi} \left(\vec{e}_i(\vec{f})\right)_k [\phi_j, F_k] = A_{ki} \left(A^{-1}\right)_{jk} = \delta_{ij}.$$

These I_i are the action variables, which are functions of the original set F_j of integrals of the motion, and therefore are themselves integrals of the motion. In action-angle variables the motion is very simple, with $\vec{I}$

constant and $\dot{\vec{\phi}} = \vec{\omega} = \text{constant}$. This is called **conditionally periodic motion**, and the ω_i are called the frequencies. If all the ratios of the ω_i's are rational, the motion will be truly periodic, with a period the least common multiple of the individual periods $2\pi/\omega_i$. More generally, there may be some relations

$$\sum_i k_i \omega_i = 0$$

for integer values k_i. Each of these is called a **relation among the frequencies**. If there are no such relations the frequencies are said to be **independent frequencies**.

In the space of possible values of $\vec{\omega}$, the subspace of values for which the frequencies are independent is surely dense. In fact, most such points have independent frequencies. We should be able to say then that most of the invariant tori $\mathcal{M}_{\vec{f}}$ have independent frequencies if the mapping $\vec{\omega}(\vec{f})$ is one-to-one. This condition is

$$\det\left(\frac{\partial\vec{\omega}}{\partial\vec{f}}\right) \neq 0, \quad \text{or equivalently} \quad \det\left(\frac{\partial\vec{\omega}}{\partial\vec{I}}\right) \neq 0.$$

When this condition holds the system is called a **nondegenerate system**. As $\omega_i = \partial H/\partial I_i$, this condition can also be written as $\det \partial^2 H/\partial_{I_i}\partial_{I_j} \neq 0$.

Consider a function g on $\mathcal{M}_{\vec{f}}$. We define two averages of this function. One is the time average we get starting at a particular point $\vec{\phi}_0$ and averaging over over an infinitely long time,

$$\langle g\rangle_t(\vec{\phi}_0) = \lim_{T\to\infty}\frac{1}{T}\int_0^T g(\vec{\phi}_0 + \vec{\omega}t)dt.$$

We may also define the average over phase space, that is, over all values of $\vec{\phi}$ describing the submanifold $\mathcal{M}_{\vec{f}}$,

$$\langle g\rangle_{\mathcal{M}_{\vec{f}}} = (2\pi)^{-n}\int_0^{2\pi}\ldots\int_0^{2\pi} g(\vec{\phi})d\phi_1\ldots d\phi_n,$$

where we have used the simple measure $d\phi_1\ldots d\phi_n$ on the space $\mathcal{M}_{\vec{f}}$. Then an important theorem states that, if the frequencies are independent, and g is a continuous function on $\mathcal{M}_{\vec{f}}$, the time and space

averages of g are the same. Note any such function g can be expanded in a Fourier series, $g(\vec{\phi}) = \sum_{\vec{k}\in\mathbb{Z}^n} g_{\vec{k}} e^{i\vec{k}\cdot\vec{\phi}}$, with $\langle g\rangle_{\mathcal{M}_{\vec{f}}} = g_{\vec{0}}$, while

$$\begin{aligned}\langle g\rangle_t &= \lim_{T\to\infty}\frac{1}{T}\int_0^T \sum_{\vec{k}} g_{\vec{k}}\, e^{i\vec{k}\cdot\vec{\phi}_0 + i\vec{k}\cdot\vec{\omega}t} dt \\ &= g_{\vec{0}} + \sum_{\vec{k}\neq\vec{0}} g_{\vec{k}}\, e^{i\vec{k}\cdot\vec{\phi}_0} \lim_{T\to\infty}\frac{1}{T}\int_0^T e^{i\vec{k}\cdot\vec{\omega}t} dt = g_{\vec{0}},\end{aligned}$$

because

$$\lim_{T\to\infty}\frac{1}{T}\int_0^T e^{i\vec{k}\cdot\vec{\omega}t} = \lim_{T\to\infty}\frac{1}{T}\frac{e^{i\vec{k}\cdot\vec{\omega}T}-1}{i\vec{k}\cdot\vec{\omega}} = 0,$$

as long as the denominator does not vanish. It is this requirement that $\vec{k}\cdot\vec{\omega}\neq 0$ for all nonzero $\vec{k}\in\mathbb{Z}^n$, which requires the frequencies to be independent.

As an important corrolary of this theorem, when it holds the trajectory is dense in $\mathcal{M}_{\vec{f}}$, and uniformly distributed, in the sense that the time spent in each specified volume of $\mathcal{M}_{\vec{f}}$ is proportional to that volume, independent of the position or shape of that volume.

If instead of independence we have relations among the frequencies, these relations, each given by a $\vec{k}\in\mathbb{Z}^n$, form a subgroup of $\mathbb{Z}^n$ (an additive group of translations by integers along each of the axes). Each such $\vec{k}$ gives a constant of the motion, $\vec{k}\cdot\vec{\phi}$. Each independent relation among the frequencies therefore restricts the dimensionality of the motion by an additional dimension, so if the subgroup is generated by r such independent relations, the motion is restricted to a manifold of reduced dimension $n-r$, and the motion on this reduced torus T^{n-r} is conditionally periodic with $n-r$ independent frequencies. The theorem and corrolaries just discussed then apply to this reduced invariant torus, but not to the whole n-dimensional torus with which we started. In particular, $\langle g\rangle_t(\phi_0)$ can depend on ϕ_0 as it varies from one submanifold T^{n-r} to another, but not along paths on the same submanifold.

If the system is nondegenerate, for typical $\vec{I}$ the ω_i's will have no relations and the invariant torus will be densely filled by the motion of the system. Therefore the invariant tori are uniquely defined, although the choices of action and angle variables is not. In the degenerate case the motion of the system does not fill the n dimensional invariant torus,

so it need not be uniquely defined. This is what happens, for example, for the two dimensional harmonic oscillator or for the Kepler problem.

7.2 Canonical Perturbation Theory

We now consider a problem with a conserved Hamiltonian which is in some sense approximated by an integrable system with n degrees of freedom. This integrable system is described with a Hamiltonian $H^{(0)}$, and we assume we have described it in terms of its action variables $I_i^{(0)}$ and angle variables $\phi_i^{(0)}$. This system is called the **unperturbed system**, and the Hamiltonian is, of course, independent of the angle variables, $H^{(0)}\left(\vec{I}^{(0)}, \vec{\phi}^{(0)}\right) = H^{(0)}\left(\vec{I}^{(0)}\right)$.

The action-angle variables of the unperturbed system are a canonical set of variables for the phase space, which is still the same phase space for the full system. We write the Hamiltonian of the full system as

$$H\left(\vec{I}^{(0)}, \vec{\phi}^{(0)}\right) = H^{(0)}\left(\vec{I}^{(0)}\right) + \epsilon H_1\left(\vec{I}^{(0)}, \vec{\phi}^{(0)}\right). \tag{7.1}$$

We have included the parameter ϵ so that we may regard the terms in H_1 as fixed in strength relative to each other, and still consider a series expansion in ϵ, which gives an overall scale to the smallness of the perturbation.

We might imagine that if the perturbation is small, there are some new action-angle variables I_i and ϕ_i for the full system, which differ by order ϵ from the unperturbed coordinates. These are new canonical coordinates, and may be generated by a generating function (of type 2),

$$F\left(\vec{I}, \vec{\phi}^{(0)}\right) = \sum \phi_i^{(0)} I_i + \epsilon F_1\left(\vec{I}, \vec{\phi}^{(0)}\right) + ...$$

This is a time-independent canonical transformation, so the full Hamiltonian is the same function on phase-space whether the unperturbed or full action-angle variables are used, but has a different functional form,

$$\tilde{H}(\vec{I}, \vec{\phi}) = H\left(\vec{I}^{(0)}, \vec{\phi}^{(0)}\right). \tag{7.2}$$

Note that the phase space itself is described periodically by the coordinates $\vec{\phi}^{(0)}$, so the Hamiltonian perturbation H_1 and the generating

function F_1 are periodic functions (with period 2π) in these variables. Thus we can expand them in Fourier series:

$$H_1\left(\vec{I}^{(0)},\vec{\phi}^{(0)}\right) = \sum_{\vec{k}} H_{1\vec{k}}\left(\vec{I}^{(0)}\right) e^{i\vec{k}\cdot\vec{\phi}^{(0)}}, \tag{7.3}$$

$$F_1\left(\vec{I},\vec{\phi}^{(0)}\right) = \sum_{\vec{k}} F_{1\vec{k}}\left(\vec{I}\right) e^{i\vec{k}\cdot\vec{\phi}^{(0)}}, \tag{7.4}$$

where the sum is over all n-tuples of integers $\vec{k}\in\mathbb{Z}^n$. The zeros of the new angles are arbitrary for each $\vec{I}$, so we may choose $F_{1\vec{0}}(I)=0$.

The unperturbed action variables, on which H_0 depends, are the old momenta given by $I_i^{(0)} = \partial F/\partial\phi_i^{(0)} = I_i + \epsilon\partial F_1/\partial\phi_i^{(0)} + ...$, so to first order

$$\begin{aligned} H_0\left(\vec{I}^{(0)}\right) &= H_0\left(\vec{I}\right) + \epsilon\sum_j \frac{\partial H_0}{\partial I_j^{(0)}}\frac{\partial F_1}{\partial\phi_j^{(0)}} + ... \\ &= H_0\left(\vec{I}\right) + \epsilon\sum_j \omega_j^{(0)}\sum_{\vec{k}} ik_j F_{1\vec{k}}(\vec{I}) e^{i\vec{k}\cdot\vec{\phi}^{(0)}} + ..., \end{aligned} \tag{7.5}$$

where we have noted that $\partial H_0/\partial I_j^{(0)} = \omega_j^{(0)}$, the frequencies of the unperturbed problem. Thus

$$\begin{aligned} \tilde{H}\left(\vec{I},\vec{\phi}\right) &= H\left(\vec{I}^{(0)},\vec{\phi}^{(0)}\right) = H^{(0)}\left(\vec{I}^{(0)}\right) + \epsilon\sum_{\vec{k}} H_{1\vec{k}}\left(\vec{I}^{(0)}\right) e^{i\vec{k}\cdot\vec{\phi}^{(0)}} \\ &= H_0\left(\vec{I}\right) + \epsilon\sum_{\vec{k}}\left(\sum_j ik_j\omega_j^{(0)} F_{1\vec{k}}(\vec{I}) + H_{1\vec{k}}\left(\vec{I}^{(0)}\right)\right) e^{i\vec{k}\cdot\vec{\phi}^{(0)}}. \end{aligned}$$

The $\vec{I}$ are the action variables of the full Hamiltonian, so $\tilde{H}(\vec{I},\vec{\phi})$ is in fact independent of $\vec{\phi}$. In the sum over Fourier modes on the right hand side, the $\phi^{(0)}$ dependence of the terms in parentheses due to the difference of $\vec{I}^{(0)}$ from $\vec{I}$ is higher order in ϵ, so the the coefficients of $e^{i\vec{k}\cdot\vec{\phi}^{(0)}}$ may be considered constants in $\phi^{(0)}$ and therefore must vanish for $\vec{k}\neq\vec{0}$. Thus the generating function is given in terms of the Hamiltonian perturbation

$$F_{1\vec{k}} = i\frac{H_{1\vec{k}}}{\vec{k}\cdot\vec{\omega}^{(0)}(\vec{I})}, \quad \vec{k}\neq\vec{0}. \tag{7.6}$$

We see that there may well be a problem in finding new action variables if there is a relation among the frequencies. If the unperturbed system is not degenerate, "most" invariant tori will have no relation among the frequencies. For these values, the extension of the procedure we have described to a full power series expansion in ϵ may be able to generate new action-angle variables, showing that the system is still integrable. That this is true for sufficiently small perturbations and "sufficiently irrational" $\omega_J^{(0)}$ is the conclusion of the famous KAM theorem.

What happens if there is a relation among the frequencies? Consider a two degree of freedom system with $p\omega_1^{(0)} + q\omega_2^{(0)} = 0$, with p and q relatively prime. Then the Euclidean algorithm shows us there are integers m and n such that $pm+qn = 1$. Instead of our initial variables $\phi_i^{(0)} \in [0, 2\pi]$ to describe the torus, we can use the linear combinations

$$\begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} = \begin{pmatrix} p & q \\ n & -m \end{pmatrix} \begin{pmatrix} \phi_1^{(0)} \\ \phi_2^{(0)} \end{pmatrix} = \mathbf{B} \cdot \begin{pmatrix} \phi_1^{(0)} \\ \phi_2^{(0)} \end{pmatrix}.$$

Then ψ_1 and ψ_2 are equally good choices for the angle variables of the unperturbed system, as $\psi_i \in [0, 2\pi]$ is a good coordinate system on the torus. The corresponding action variables are $I_i' = (B^{-1})_{ji} I_j$, and the corresponding new frequencies are

$$\omega_i' = \frac{\partial H}{\partial I_i'} = \sum_j \frac{\partial H}{\partial I_j} \frac{\partial I_j}{\partial I_i'} = B_{ij}\omega_j^{(0)},$$

and so in particular $\omega_1' = p\omega_1^{(0)} + q\omega_2^{(0)} = 0$ on the chosen invariant torus. This conclusion is also obvious from the equations of motion $\dot{\phi}_i = \omega_i$.

In the unperturbed problem, on our initial invariant torus, ψ_1 is a constant of the motion, so in the perturbed system we might expect it to vary slowly with respect to ψ_2. Then it is appropriate to use the adiabatic approximation

7.2.1 Time Dependent Perturbation Theory

Consider a problem for which the Hamiltonian is approximately that of an exactly solvable problem. For example, let's take the pendulum,

$L = \frac{1}{2}m\ell^2\dot{\theta}^2 - mg\ell(1-\cos\theta)$, $p_\theta = m\ell^2\dot{\theta}$, $H = p_\theta^2/2m\ell^2 + mg\ell(1-\cos\theta) \approx p_\theta^2/2m\ell^2 + \frac{1}{2}mg\ell\theta^2$, which is approximately given by an harmonic oscillator if the excursions are not too big. More generally

$$H(q,p,t) = H_0(q,p,t) + \epsilon H_I(q,p,t),$$

where $\epsilon H_I(q,p,t)$ is considered a small "interaction" Hamiltonian. We assume we know Hamilton's principal function $S_0(q,P,t)$ for the unperturbed problem, which gives a canonical transformation $(q,p) \to (Q,P)$, and in the limit $\epsilon \to 0$, $\dot{Q} = \dot{P} = 0$. For the full problem,

$$K(Q,P,t) = H_0 + \epsilon H_I + \frac{\partial S_0}{\partial t} = \epsilon H_I,$$

and is small. Expressing H_I in terms of the new variables (Q,P), we have that

$$\dot{Q} = \epsilon\frac{\partial H_I}{\partial P}, \qquad \dot{P} = -\epsilon\frac{\partial H_I}{\partial Q}$$

and these are slowly varying because ϵ is small. In symplectic form, with $\zeta^T = (Q,P)$, we have, of course,

$$\dot{\zeta} = \epsilon J\cdot\nabla H_I(\zeta). \tag{7.7}$$

This differential equation can be solved perturbatively. If we assume an expansion

$$\zeta(t) = \zeta_0(t) + \epsilon\zeta_1(t) + \epsilon^2\zeta_2(t) + ...,$$

$\dot{\zeta}_n$ on the left of (7.7) can be determined from only lower order terms in ζ on the right hand side, so we can recursively find higher and higher order terms in ϵ. This is a good expansion for ϵ small for fixed t, but as we are making an error of some order, say m, in $\dot{\zeta}$, this is $\mathcal{O}(\epsilon^m t)$ for $\zeta(t)$. Thus for calculating the long time behavior of the motion, this method is unlikely to work in the sense that any finite order calculation cannot be expected to be good for $t \to \infty$. Even though H and H_0 differ only slightly, and so acting on any given η they will produce only slightly different rates of change, as time goes on there is nothing to prevent these differences from building up. In a periodic motion, for example, the perturbation is likely to make a change $\Delta\tau$ of order ϵ in the period τ of the motion, so at a time $t \sim \tau^2/2\Delta\tau$ later, the systems will be at opposite sides of their orbits, not close together at all.

7.3 Adiabatic Invariants

7.3.1 Introduction

We are going to discuss the evolution of a system which is, at every instant, given by an integrable Hamiltonian, but for which the parameters of that Hamiltonian are slowly varying functions of time. We will find that this leads to an approximation in which the actions are time invariant. We begin with a qualitative discussion, and then we discuss a formal perturbative expansion.

First we will consider a system with one degree of freedom described by a Hamiltonian $H(q,p,t)$ which has a slow time dependence. Let us call T_V the time scale over which the Hamiltonian has significant variation (for fixed q,p). For a short time interval $<< T_V$, such a system could be approximated by the Hamiltonian $H_0(q,p) = H(q,p,t_0)$, where t_0 is a fixed time within that interval. Any perturbative solution based on this approximation may be good during this time interval, but if extended to times comparable to the time scale T_V over which $H(q,p,t)$ varies, the perturbative solution will break down. We wish to show, however, that if the motion is bound and the period of the motion determined by H_0 is much less than the time scale of variations T_V, the action is very nearly conserved, even for evolution over a time interval comparable to T_V. We say that the action is an **adiabatic invariant**.

7.3.2 For a time-independent Hamiltonian

In the absence of any explicit time dependence, a Hamiltonian is conserved. The motion is restricted to lie on a particular contour $H(q,p) = \alpha$, for all times. For bound solutions to the equations of motion, the solutions are periodic closed orbits in phase space. We will call this contour Γ, and the period of the motion τ. Let us parameterize the contour with the **action-angle** variable ϕ. We take an arbitrary point on Γ to be $\phi = 0$ and also $(q(0), p(0))$. Every other point is determined by $\Gamma(\phi) = (q(\phi\tau/2\pi), p(\phi\tau/2\pi))$, so the complete orbit is given by $\Gamma(\phi), \phi \in [0, 2\pi)$. The action is defined as

$$J = \frac{1}{2\pi} \oint p dq. \tag{7.8}$$

This may be considered as an integral along one cycle in extended phase space, $2\pi J(t) = \int_t^{t+\tau} p(t')\dot{q}(t')dt'$. Because $p(t)$ and $\dot{q}(t)$ are periodic with period τ, J is independent of time t. But J can also be thought of as an integral in phase space itself, $2\pi J = \oint_\Gamma p dq$, of a one form $\omega_1 = pdq$ along the closed path $\Gamma(\phi)$, $\phi \in [0, 2\pi]$, which is the orbit in question. By Stokes' Theorem,

$$\int_S d\omega = \int_{\delta S} \omega,$$

true for any n-form ω and region S of a manifold, we have $2\pi J = \int_A dp \wedge dq$, where A is the area bounded by Γ.

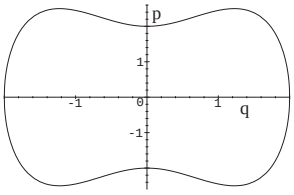


Fig. 1. The orbit of an autonomous system in phase space.

In extended phase space $\{q, p, t\}$, if we start at time t=0 with any point (q, p) on Γ, the trajectory swept out by the equations of motion, $(q(t), p(t), t)$ will lie on the surface of a cylinder with base A extended in the time direction. Let Γ_t be the embedding of Γ into the time slice at t, which is the intersection of the cylinder with that time slice. The surface of the cylinder can also be viewed as the set of all the dynamical trajectories which start on Γ at $t = 0$. In other words, if $\mathcal{T}_\phi(t)$ is the trajectory of the system which starts at $\Gamma(\phi)$ at t=0, the set of $\mathcal{T}_\phi(t)$ for $\phi \in [0, 2\pi]$, $t \in [0, T]$, sweeps out the same surface as Γ_t, $t \in [0, T]$. Because this is an autonomous system, the value of the action J is the same, regardless of whether it is evaluated along Γ_t, for any t, or evaluated along one period for any of the trajectories starting on Γ_0. If we terminate the evolution at time T, the end of the cylinder, Γ_T, is the same orbit of the motion, in phase space, as was Γ_0.

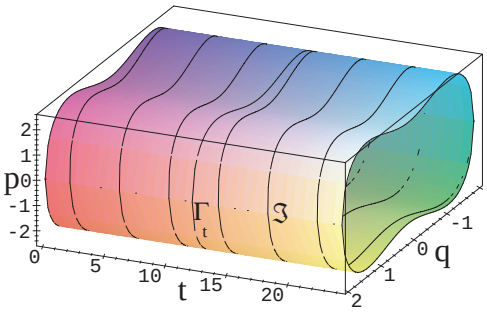


Fig 2. The surface in extended phase space, generated by the ensemble of systems which start at time $t = 0$ on the orbit Γ shown in Fig. 1. One such trajectory is shown, labelled $\mathcal{I}$, and also shown is one of the Γ_t.

7.3.3 Slow time variation in $H(q, p, t)$

Now consider a time dependent Hamiltonian $H(q, p, t)$. For a short interval of time near t_0, if we assume the time variation of H is slowly varying, the autonomous Hamiltonian $H(q, p, t_0)$ will provide an approximation, one that has conserved energy and bound orbits given by contours of that energy. Consider extended phase space, and a closed path $\Gamma_0(\phi)$ in the t=0 plane which is a contour of $H(q, p, 0)$, just as we had in the time-independent case. For each point ϕ on this path, construct the trajectory $\mathcal{T}_\phi(t)$ evolving from $\Gamma(\phi)$ under the influence of the **full** Hamiltonian $H(q, p, t)$, up until some fixed final time $t = T$. This collection of trajectories will sweep out a curved surface Σ_1 with boundary Γ_0 at t=0 and another we call Γ_T at time t=T. Because the Hamiltonian does change with time, these Γ_t, the intersections of Σ_1 with the planes at various times t, are not congruent. Let Σ_0 and Σ_T be the regions of the t=0 and t=T planes bounded by Γ_0 and Γ_T respectively, oriented so that their normals go forward in time.

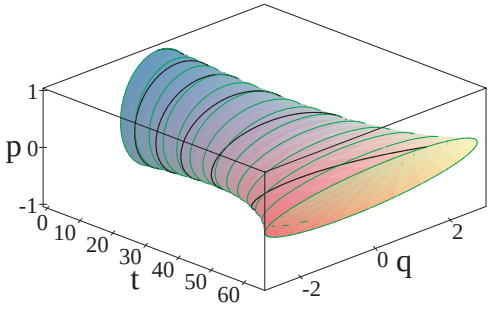


Fig. 3. The motion of a harmonic oscillator with time-varying spring constant $k \propto (1 - \epsilon t)^4$, with $\epsilon = 0.01$. [Note that the horn is not tipping downwards, but the surface ends flat against the $t = 65$ plane.]

This constructs a region which is a deformation of the cylinder[1] that we had in the case where H was independent of time. If the variation of H is slow on a time scale of T, the path Γ_T will not differ much from Γ_0, so it will be nearly an orbit and the action defined by $\oint p dq$ around Γ_T will be nearly that around Γ_0. We shall show something much stronger; that if the time dependence of H is a slow variation compared with the approximate period of the motion, then each Γ_t is nearly an orbit and the action on that path, $\tilde{J}(t) = \oint_{\Gamma_t} p dq$ is constant, even if the Hamiltonian varies considerably over time T.

[1] Of course it is possible that after some time, which must be on a time scale of order T_V rather than the much shorter cycle time τ, the trajectories might intersect, which would require the system to reach a critical point in phase space. We assume that our final time T is before the system reaches a critical point.

The Σ's form a closed surface, which is $\Sigma_1 + \Sigma_T - \Sigma_0$, where we have taken the orientation of Σ_1 to point outwards, and made up for the inward-pointing direction of Σ_0 with a negative sign. Call the volume enclosed by this closed surface V.

We will first show that the actions $\tilde{J}(0)$ and $\tilde{J}(T)$ defined on the ends of the cylinder are the same. Again from Stokes' theorem, they are

$$\tilde{J}(0) = \int_{\Gamma_0} pdq = \int_{\Sigma_0} dp \wedge dq \quad \text{and} \quad \tilde{J}(T) = \int_{\Sigma_T} dp \wedge dq$$

respectively. Each of these surfaces has no component in the t direction, so we may also evaluate $\tilde{J}(t) = \int_{\Sigma_t} \omega_2$, where

$$\omega_2 = dp \wedge dq - dH \wedge dt. \tag{7.9}$$

Clearly ω_2 is closed, $d\omega_2 = 0$, as ω_2 is a sum of wedge products of closed forms.

As H is a function on extended phase space, $dH = \frac{\partial H}{\partial p}dp + \frac{\partial H}{\partial q}dq + \frac{\partial H}{\partial t}dt$, and thus

$$\begin{aligned} \omega_2 &= dp \wedge dq - \frac{\partial H}{\partial p}dp \wedge dt - \frac{\partial H}{\partial q}dq \wedge dt \\ &= \left(dp + \frac{\partial H}{\partial q}dt\right) \wedge \left(dq - \frac{\partial H}{\partial p}dt\right), \end{aligned} \tag{7.10}$$

where we have used the antisymmetry of the wedge product, $dq \wedge dt = -dt \wedge dq$, and $dt \wedge dt = 0$.

Now the interesting thing about this rewriting of the action in terms of the new form (7.10) of ω_2 is that ω_2 is now a product of two 1-forms

$$\omega_2 = \omega_a \wedge \omega_b, \quad \text{where} \quad \omega_a = dp + \frac{\partial H}{\partial q}dt, \quad \omega_b = dq - \frac{\partial H}{\partial p}dt,$$

and each of ω_a and ω_b vanishes along any trajectory of the motion, along which Hamilton's equations require

$$\frac{dp}{dt} = -\frac{\partial H}{\partial q}, \quad \frac{dq}{dt} = \frac{\partial H}{\partial p}.$$

As a consequence, ω_2 vanishes at any point when evaluated on a surface which contains a physical trajectory, so in particular ω_2 vanishes over the surface Σ_1 generated by the trajectories. Because ω_2 is closed,

$$\int_{\Sigma_1+\Sigma_T-\Sigma_0} \omega_2 = \int_V d\omega_2 = 0$$

where the first equality is due to Gauss' law, one form of the generalized Stokes' theorem. Then we have

$$\tilde{J}(T) = \int_{\Sigma_T} \omega_2 = \int_{\Sigma_0} \omega_2 = \tilde{J}(0).$$

What we have shown here for the area in phase space enclosed by an orbit holds equally well for any area in phase space. If A is a region in phase space, and if we define B as that region in phase space in which systems will lie at time $t = T$ if the system was in A at time $t = 0$, then $\int_A dp \wedge dq = \int_B dp \wedge dq$. For systems with $n > 1$ degrees of freedom, we may consider a set of n forms $(dp \wedge dq)^j, j = 1...n$, which are all conserved under dynamical evolution. In particular, $(dp \wedge dq)^n$ tells us the hypervolume in phase space is preserved under its motion under evolution according to Hamilton's equations of motion. This truth is known as Liouville's theorem, though the n invariants $(dp \wedge dq)^j$ are known as Poincaré invariants.

While we have shown that the integral $\int pdq$ is conserved when evaluated over an initial contour in phase space at time $t = 0$, and then compared to its integral over the path at time $t = T$ given by the time evolution of the ensembles which started on the first path, neither of these integrals are exactly an action.

In fact, for a time-varying system the action is not really well defined, because actions are defined only for periodic motion. For the one dimensional harmonic oscillator (with varying spring constant) of Fig. 3, a reasonable substitute definition is to define J for each "period" from one passing to the right through the symmetry point, $q = 0$, to the next such crossing. The

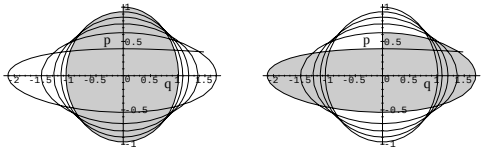


Fig. 4. The trajectory in phase space of the system in Fig. 3. The "actions" during two "orbits" are shown by shading. In the adiabatic approximation the areas are equal.

trajectory of a single such system as it moves through phase space is shown in Fig. 4. The integrals $\int p(t)dq(t)$ over time intervals between successive forward crossings of $q = 0$ is shown for the first and last such intervals. While these appear to have roughly the same area, what we have shown is that the integrals over the curves Γ_t are the same. In Fig. 5 we show Γ_t for t at the beginning of the first and fifth "periods", together with the actual motion through those periods. The deviations are of order $\epsilon\tau$ and not of ϵT, and so are negligible as long as the approximate period is small compared to $T_V \sim 1/\epsilon$.

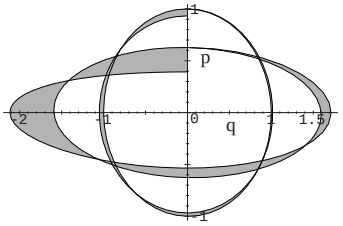


Fig. 5. The differences between the actual trajectories (thick lines) during the first and fifth oscillations, and the ensembles Γ_t at the moments of the beginnings of those periods. The area enclosed by the latter two curves are strictly equal, as we have shown. The figure indicates the differences between each of those curves and the actual trajectories.

Another way we can define an action in our time-varying problem is to write an expression for the action on extended phase space, $J(q, p, t_0)$, given by the action at that value of (q, p) for a system with hamiltonian fixed at the time in question, $H_{t_0}(q, p) := H(q, p, t_0)$. This is an ordinary harmonic oscillator with $\omega = \sqrt{k(t_0)/m}$. For an autonomous harmonic oscillator the area of the elliptical orbit is

$$2\pi J = \pi p_{\max} q_{\max} = \pi m\omega q_{\max}^2,$$

while the energy is

$$\frac{p^2}{2m} + \frac{m\omega^2}{2}q^2 = E = \frac{m\omega^2}{2}q_{\max}^2,$$

so we can write an expression for the action as a function on extended phase space,

$$J = \frac{1}{2}m\omega q_{\max}^2 = E/\omega = \frac{p^2}{2m\omega(t)} + \frac{m\omega(t)}{2}q^2.$$

With this definition, we can assign a value for the action to the system as a each time, which in the autonomous case agrees with the standard action.

From this discussion, we see that if the Hamiltonian varies slowly on the time scale of an oscillation of the system, the action will remain fairly close to the $\tilde{J}_t$, which is conserved. Thus the action is an adiabatic invariant, conserved in the limit that $\tau/T_V \to 0$.

To see how this works in a particular example, consider the harmonic oscillator with a time-varying spring constant, which we have chosen to be $k(t) = k_0(1 - \epsilon t)^4$. With $\epsilon = 0.01$, in units given by the initial ω, the evolution is shown from time 0 to time 65. During this time the spring constant becomes over 66 times weaker, and the natural frequency decreases by a factor of more than eight, as does the energy, but the action remains quite close to its original value, even though the adiabatic approximation is clearly badly violated by a spring constant which changes by a factor of more than six during the last oscillation.

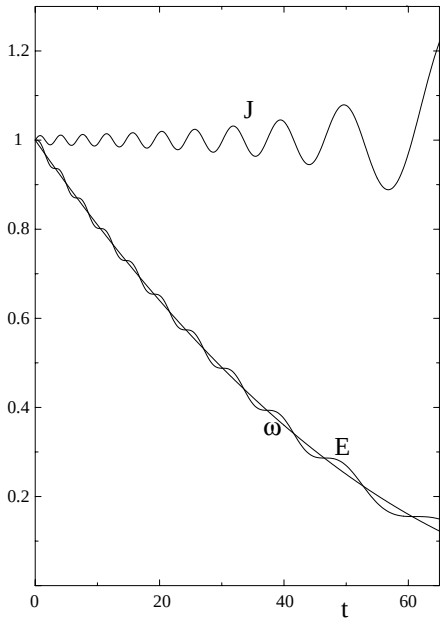


Fig. 6. The change in angular frequency, energy, and action for the time-varying spring-constant harmonic oscillator, with $k(t) \propto (1 - \epsilon t)^4$, with $\epsilon = \omega(0)/100$

We see that the failure of the action to be exactly conserved is due to the descrepancy between the action evaluated on the actual path of a single system and the action evaluated on the curve representing the evolution, after a given time, of an ensemble of systems all of which began at time $t = 0$ on a path in phase space which would have been their paths had the system been autonomous.

This might tempt us to consider a different problem, in which the time dependance of the hamiltonian varies only during a fixed time interval, $t \in [0, T]$, but is constant before $t = 0$ and after T. If we look at the motion during an oscillation before $t = 0$, the system's trajectory

projects exactly onto Γ_0, so the initial action $J = \tilde{J}(0)$. If we consider a full oscillation beginning after time T, the actual trajectory is again a contour of energy in phase space. Does this mean the action is exactly conserved?

There must be something wrong with this argument, because the constancy of $\tilde{J}(t)$ did not depend on assumptions of slow variation of the Hamiltonian. Thus it should apply to the pumped swing, and claim that it is impossible to increase the energy of the oscillation by periodic changes in the spring constant. But we know that is not correct. Examining this case will point out the flawed assumption in the argument. In Fig. 7, we show the surface generated by time evolution of an ensemble of systems initially on an energy contour for a harmonic oscillator. Starting at time 0, the spring constant is modulated by 10% at a frequency twice the natural frequency, for four natural periods. Thereafter the Hamiltonian is the same as is was before $t = 0$, and each system's path in phase space continues as a circle in phase space (in the units shown), but the ensemble of systems form a very elongated figure, rather than a circle.

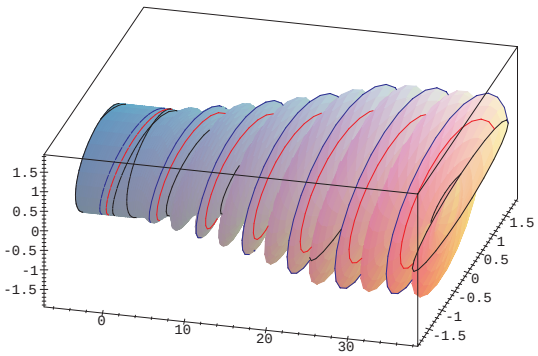


Fig. 7. The surface Σ_1 for a harmonic oscillator with a spring constant which varies, for the interval $t \in [0, 8\pi]$, as $k(t) = k(0)(1 + 0.1 \sin 2t)$.

What has happened is that some of the systems in the ensemble have gained energy from the pumping of the spring constant, while others have lost energy. Thus there has been no conservation of the action for individual systems, but rather there is some (vaguely understood) average action which is unchanged.

Thus we see what is physically the crucial point in the adiabatic expansion: if all the systems in the ensemble experience the perturba-

tion in the same way, because the time variation of the hamiltonian is slow compared to the time it takes for each system in the ensemble to occupy the initial position (in phase space) of every other system, then each system will have its action conserved.

7.3.4 Systems with Many Degrees of Freedom

In the discussion above we considered as our starting point an autonomous system with one degree of freedom. As the hamiltonian is a conserved function on phase space, this is an integrable system. For systems with $n > 1$ degrees of freedom, we wish to again start with an integrable system. Such systems have n invariant "integrals of the motion in involution", and their phase space can be described in terms of n action variables J_i and corresponding coordinates ϕ_i. Phase space is periodic in each of the ϕ_i with period 2π, and the submanifold $\mathcal{M}_{\vec{f}}$ of phase space which has a given set $\{f_i\}$ of values for the J_i is an n-dimensional torus. As the J_i are conserved, the motion is confined to $\mathcal{M}_{\vec{f}}$, and indeed the equations of motion are very simple, $d\phi_i/dt = \nu_i$ (constant). $\mathcal{M}_{\vec{f}}$ is known as an invariant torus.

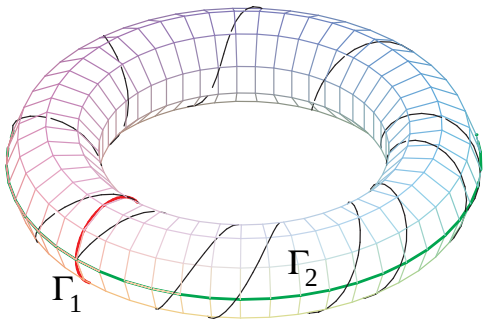


Fig 8. For an integrable system with two degrees of freedom, the motion is confined to a 2-torus, and the trajectories are uniform motion in each of the angles, with independent frequencies. The two actions J_1 and J_2 may be considered as integrals of the single 1-form $\omega_1 = \sum J_i d\phi_i$ over two independant cycles Γ_1 and Γ_2 as shown.

In the one variable case we related the action to the 1-form $p\ dq$. On the invariant torus, the actions are constants and so it is trivially true that $J_i = \oint J_i d\phi_i/2\pi$, where the integral is $\int_0^{2\pi} d\phi_i$ with the other ϕ's held fixed. This might lead one to think about n 1-forms without a sum, but it is more profitable to recognize that the single 1-form $\omega_1 = \sum J_i d\phi_i$ alone contains all of the information we need. First note that, restricted to $\mathcal{M}_{\vec{f}}$, dJ_i vanishes, so ω_1 is closed, and its integral is a topological invariant, that is, unchanged under continuous deformations of the path. We can take a set

of paths, or cycles, Γ_i, each winding around the torus only in the ϕ_i direction, and we then have $J_i = \frac{1}{2\pi}\int_{\Gamma_i}\omega_1$. The answer is completely independent of where the path Γ_i is drawn on $\mathcal{M}_{\vec{f}}$, as long as its topology is unchanged. Thus the action can be thought of as a function on the simplicial homology H_1 of $\mathcal{M}_{\vec{f}}$. The actions can also be expressed as an integral over a surface Σ_i bounded by the Γ_i, $J_i = \frac{1}{2\pi}\int_{\Sigma_i}\sum dJ_i \wedge d\phi_i$. Notice that this surface does not lie on the invariant torus but cuts across it. This formulation has two advantages. First, $\sum dp_i \wedge dq_i$ is invariant under arbitrary canonical transformations, so $\sum dJ_i \wedge d\phi_i$ is just one way to write it. Secondly, on a surface of constant t, such as Σ_i, it is identical to the fundamental form

$$\omega_2 = \sum_{i=1}^{n} dp_i \wedge dq_i - dH \wedge dt,$$

the generalization to several degrees of freedom of the form we used to show the invariance of the integral under time evolution in the single degree of freedom case.

Now suppose that our system is subject to some time-dependent perturbation, but that at all times its Hamiltonian remains close to an integrable system, though that system might have parameters which vary with time. Let's also assume that after time T the hamiltonian again becomes an autonomous integrable system, though perhaps with parameters different from what it had at $t = 0$.

Consider the evolution in time, under the full hamiltonian, of each system which at $t = 0$ was at some point $\vec{\phi}_0$ on the invariant torus $\mathcal{M}_{\vec{f}}$ of the original unperturbed system. Follow each such system until time T. We assume that none of these systems reaches a critical point during this evolution. The region in phase space thus varies continuously, and at the fixed later time T, it still will be topologically an n-torus, which we will call $\mathcal{B}$. The image of each of the cycles Γ_i will be a cycle $\tilde{\Gamma}_i$ on $\mathcal{B}$, and together these images will be a a basis of the homology H_1 of the $\mathcal{B}$. Let $\tilde{\Sigma}_i$ be surfaces within the $t = T$ hyperplane bounded by $\tilde{\Gamma}_i$. Define $\tilde{J}_i$ to be the

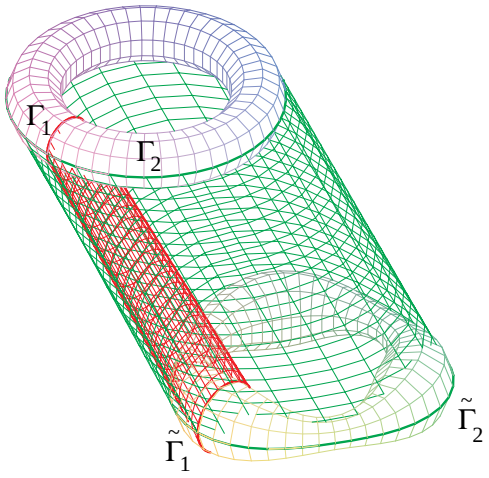


Fig. 9. Time evolution of the invariant torus, and each of two of the cycles on it.

integral on $\tilde{\Sigma}_i$ of ω_2, so $\tilde{J}_i = \frac{1}{2\pi} \int_{\tilde{\Sigma}_i} \sum_j dp_j \wedge dq_j$, where we can drop the $dH \wedge dt$ term on a constant t surface, as $dt = 0$. We can now repeat the argument from the one-degree-of-freedom case to show that the integrals $\tilde{J}_i = J_i$, again because ω_2 is a closed 2-form which vanishes on the surface of evolution, so that its integrals on the end-caps are the same.

Now we have assumed that the system is again integrable at $t = T$, so there are new actions J'_i, and new invariant tori

$$\mathcal{M}'_{\vec{g}} = \{(\vec{q}, \vec{p}) \ni J'_i(\vec{q}, \vec{p}) = g_i\}.$$

Each initial system which started at $\vec{\phi}_0$ winds up on some new invariant torus with $\vec{g}(\vec{\phi}_0)$.

If the variation of the hamiltonian is sufficiently slow and smoothly varying on phase space, and if the unperturbed motion is sufficiently ergotic that each system samples the full invariant torus on a time scale short compared to the variation time of the hamiltonian, then each initial system $\vec{\phi}_0$ may be expected to wind up with the same values of the perturbed actions, so $\vec{g}$ is independant of $\vec{\phi}_0$. That means that the torus $\mathcal{B}$ is, to some good approximation, one of the invariant tori $\mathcal{M}'_{\vec{g}}$,

that the cycles of $\mathcal{B}$ are cycles of $\mathcal{M}'_{\vec{g}}$, and therefore that $J'_i = \tilde{J}_i = J_i$, and each of the actions is an adiabatic invariant.

7.3.5 Formal Perturbative Treatment

Consider a system based on a system $H(\vec{q}, \vec{p}, \vec{\lambda})$, where $\vec{\lambda}$ is a set of parameters, which is integrable for each constant value of $\vec{\lambda}$ within some domain of interest. Now suppose our "real" system is described by the same Hamiltonian, but with $\vec{\lambda}(t)$ a given slowly varying function of time. Although the full Hamiltonian is not invariant, we will show that the action variables are approximately so.

For each fixed value of $\vec{\lambda}$, there is a generating function of type 1 to the corresponding action-angle variables:

$$F_1(\vec{q}, \vec{\phi}, \vec{\lambda}) : (\vec{q}, \vec{p}) \to (\vec{\phi}, \vec{I}).$$

This is a time-independent transformation, so the Hamiltonian may be written as $H(\vec{I}(\vec{q}, \vec{p}), \vec{\lambda})$, independent of the angle variable. This constant $\vec{\lambda}$ Hamiltonian has equations of motion $\dot{\phi}_i = \partial H/\partial I_i = \omega_i(\vec{\lambda}), \dot{I}_i = 0$. But in the case where $\vec{\lambda}$ is a function of time, the transformation F_1 is not a time-independent one, so the correct Hamiltonian is not just the reexpressed Hamiltonian but has an additional term

$$K(\vec{\phi}, \vec{I}, \vec{\lambda}) = H(\vec{I}, \vec{\lambda}) + \sum_n \frac{\partial F_1}{\partial \lambda_n} \frac{d\lambda_n}{dt},$$

where the second term is the expansion of $\partial F_1/\partial t$ by the chain rule. The equations of motion involve differentiating K with respect to one of the variables (ϕ_j, I_j) holding the others, and time, fixed. While these are not the usual variables $(\vec{q}, \vec{\phi})$ for F_1, they are coordinates of phase space, so F_1 can be expressed in terms of (ϕ_j, I_j), and as shown in (**??**), it is periodic in the ϕ_j. The equation of motion for I_j is

$$\begin{aligned} \dot{\phi}_i &= \omega_i(\vec{\lambda}) + \sum_n \frac{\partial^2 F_1}{\partial \lambda_n \partial I_i} \dot{\lambda}_n, \\ \dot{I}_i &= \sum_n \frac{\partial^2 F_1}{\partial \lambda_n \partial \phi_i} \dot{\lambda}_n, \end{aligned}$$

where all the partial derivatives are with respect to the variables $\vec{\phi}, \vec{I}, \vec{\lambda}$. We first note that if the parameters λ are slowly varying, the $\dot{\lambda}_n$'s in the equations of motion make the deviations from the unperturbed system small, of first order in $\epsilon/\tau = \dot{\lambda}/\lambda$, where τ is a typical time for oscillation of the system. But in fact the constancy of the action is better than that, because the expression for $\dot{I}_j$ is predominantly an oscillatory term with zero mean. This is most easily analyzed when the unperturbed system is truly periodic, with period τ. Then during one period $t \in [0, \tau]$, $\dot{\lambda}(t) \approx \dot{\lambda}(0) + t\ddot{\lambda}$. Assuming $\lambda(t)$ varies smoothly on a time scale τ/ϵ, $\ddot{\lambda} \sim \lambda\mathcal{O}(\epsilon^2/\tau^2)$, so if we are willing to drop terms of order ϵ^2, we may treat $\dot{\lambda}$ as a constant. We can then also evaluate F_1 on the orbit of the unperturbed system, as that differs from the true orbit by order ϵ, and the resulting value is multiplied by $\dot{\lambda}$, which is already of order ϵ/τ, and the result is to be integrated over a period τ. Then we may write the change of I_j over one period as

$$\Delta I_j \approx \sum_n \dot{\lambda}_n \int_0^\tau \frac{\partial}{\partial \phi_j}\left(\frac{\partial F_1}{\partial \lambda_n}\right) dt.$$

But F_1 is a well defined single-valued function on the invariant manifold, and so are its derivatives with respect to λ_n, so we may replace the time integral by an integral over the orbit,

$$\Delta I_j \approx \sum_n \dot{\lambda}_n \frac{\tau}{L} \oint \frac{\partial}{\partial \phi_j}\left(\frac{\partial F_1}{\partial \lambda_n}\right) d\phi_j = 0,$$

where L is the length of the orbit, and we have used the fact that for the unperturbed system $d\phi_j/dt$ is constant.

Thus the action variables have oscillations of order ϵ, but these variations do not grow with time. Over a time t, $\Delta\vec{I} = \mathcal{O}(\epsilon) + t\mathcal{O}(\epsilon^2/\tau)$, and is therefore conserved up to order ϵ even for times as large as τ/ϵ, corresponding to many natural periods, and also corresponding to the time scale on which the Hamiltonian is varying significantly.

This form of perturbation, corresponding to variation of constants on a time scale slow compared to the natural frequencies of the unperturbed system, is known as an adiabatic variation, and a quantity conserved to order ϵ over times comparable to the variation itself is called an **adiabatic invariant**. Classic examples include ideal

gases in a slowly varying container, a pendulum of slowly varying length, and the motion of a rapidly moving charged particle in a strong but slowly varying magnetic field. It is interesting to note that in Bohr-Sommerfeld quantization in the old quantum mechanics, used before the Schrödinger equation clarified such issues, the quantization of bound states was related to quantization of the action. For example, in Bohr theory the electrons are in states with action nh, with n a positive integer and h Planck's constant. Because these values are preserved under adiabatic perturbation, it is possible that an adiabatic perturbation of a quantum mechanical system maintains the system in the initial quantum mechanical state, and indeed this can be shown, with the full quantum theory, to be the case in general. An important application is cooling by adiabatic demagnetization. Here atoms with a magnetic moment are placed in a strong magnetic field and reach equilibrium according to the Boltzman distribution for their polarizations. If the magnetic field is adiabatically reduced, the separation energies of the various polarization states is reduced proportionally. As the distribution of polarization states remains the same for the adiabatic change, it now fits a Boltzman distribution for a temperature reduced proportionally to the field, so the atoms have been cooled.

7.4 Rapidly Varying Perturbations

At the other extreme from adiabatic perturbations, we may ask what happens to a system if we add a perturbative potential which oscillates rapidly with respect to the natural frequencies of the unperturbed system. If the forces are of the same magnitude as those of the unperturbed system, we would expect that the coordinates and momenta would change little during the short time of one external oscillation, and that the effects of the force might be little more than adding jitter to the unperturbed motion. Consider the case that the external force is a pure sinusoidal oscillation,

$$H(\vec{q},\vec{p}) = H_0(\vec{q},\vec{p}) + U(\vec{q})\sin\omega t,$$

and let us write the resulting motion as

$$\vec{q}(t) \;=\; \bar{q}(t) + \vec{\xi}(t),$$

$$\vec{p}(t) \;=\; \bar{p}(t) + \vec{\eta}(t),$$

where we subtract out the average smoothly varying functions $\bar{q}$ and $\bar{p}$, leaving the rapidly oscillating pieces $\vec{\xi}$ and $\vec{\eta}$, which have natural time scales of $2\pi/\omega$. Thus $\ddot{\xi}, \omega\dot{\xi}, \omega^2\xi, \dot{\eta}$ and $\omega\eta$ should all remain finite as ω gets large with all the parameters of H_0 and $U(q)$ fixed. The equations of motion are

$$\begin{aligned}
\dot{\bar{q}}_j + \dot{\xi}_j &= \frac{\partial H_0}{\partial p_j}(\vec{q},\vec{p}) \\
&= \frac{\partial H_0}{\partial p_j}(\bar{q},\bar{p}) + \sum_k \xi_k \frac{\partial^2 H_0}{\partial p_j \partial q_k}(\bar{q},\bar{p}) + \sum_k \eta_k \frac{\partial^2 H_0}{\partial p_j \partial p_k}(\bar{q},\bar{p}) \\
&\quad + \frac{1}{2}\sum_{k\ell} \eta_k \eta_\ell \frac{\partial^3 H_0}{\partial p_j \partial p_k \partial p_\ell}(\bar{q},\bar{p}) + \mathcal{O}(\omega^{-3}) \\
\dot{\bar{p}}_j + \dot{\eta}_j &= -\frac{\partial H_0}{\partial q_j}(\vec{q},\vec{p}) - \frac{\partial U}{\partial q_j}\sin\omega t \\
&= -\frac{\partial H_0}{\partial q_j}(\bar{q},\bar{p}) - \sum_k \xi_k \frac{\partial^2 H_0}{\partial q_j \partial q_k}(\bar{q},\bar{p}) - \sum_k \eta_k \frac{\partial^2 H_0}{\partial q_j \partial p_k}(\bar{q},\bar{p}) \\
&\quad - \frac{1}{2}\sum_{k\ell} \eta_k \eta_\ell \frac{\partial^3 H_0}{\partial q_j \partial p_k \partial p_\ell}(\bar{q},\bar{p}) - \sin\omega t \frac{\partial U}{\partial q_j}(\bar{q}) \\
&\quad - \sum_k \xi_k \sin\omega t \frac{\partial^2 U}{\partial q_j \partial q_k}(\bar{q}) + \mathcal{O}(\omega^{-3}).
\end{aligned} \tag{7.11}$$

Averaging over one period, ignoring the changes in the slowly varying functions[2] of $\bar{q}$ and $\bar{p}$, making use of the assumption that the average

[2]The careful reader will note that the argument is not really valid, because we have variations in the coefficient of η of order ω^{-1} and in the coefficient of $\sin\omega t$ of order ω^{-2}. A valid argument concludes first that Eqs (7.12) are correct through order ω^{-1}, which is then enough to get Eqs. (7.13) to the order stated, and hence (7.14) and (7.15), with the assumption that any additional terms are rapidly oscillating. If we then average (7.11) over a period centered at $2\pi n/\omega$, the expressions which we claimed vanished do, except that the averages

$$\langle \dot{\eta}_j \rangle = \langle -\sin\omega t \frac{\partial U}{\partial q_j} \rangle = -\frac{\partial}{\partial t}\frac{\partial U}{\partial q_j},$$

cancelling the inaccuracies of our argument.

of $\vec{\xi}$ and of $\vec{\eta}$ vanish, and dropping terms of order ω^{-3}, we have

$$\begin{aligned}
\dot{\bar{q}}_j &= \frac{\partial H_0}{\partial p_j}(\bar{q},\bar{p}) + \frac{1}{2}\sum_{k\ell}\langle\eta_k\eta_\ell\rangle\frac{\partial^3 H_0}{\partial p_j\partial p_k\partial p_\ell}(\bar{q},\bar{p}),\\
\dot{\bar{p}}_j &= -\frac{\partial H_0}{\partial q_j}(\bar{q},\bar{p}) - \sum_k\langle\xi_k\sin\omega t\rangle\frac{\partial^2 U}{\partial q_j\partial q_k}(\bar{q}) \\
&\quad -\frac{1}{2}\sum_{k\ell}\langle\eta_k\eta_\ell\rangle\frac{\partial^3 H_0}{\partial q_j\partial p_k\partial p_\ell}(\bar{q},\bar{p}).
\end{aligned} \tag{7.12}$$

Plugging these equations back into 7.11 to evaluate $\dot{\xi}$ and $\dot{\eta}$ to lowest order gives

$$\begin{aligned}
\dot{\xi}_j &= \sum_k \eta_k\frac{\partial^2 H_0}{\partial\bar{p}_k\partial\bar{p}_j} + \mathcal{O}(\omega^{-2}),\\
\dot{\eta}_j &= -\sin\omega t\frac{\partial U}{\partial\bar{q}_j} + \mathcal{O}(\omega^{-2}).
\end{aligned} \tag{7.13}$$

Integrating first

$$\eta_j(t) = \frac{1}{\omega}\frac{\partial U(\bar{q})}{\partial\bar{q}_j}\cos\omega t - \frac{1}{\omega^2}\sin\omega t\frac{\partial}{\partial t}\frac{\partial U}{\partial\bar{q}_j} + \mathcal{O}(\omega^{-3}). \tag{7.14}$$

Then integrating for ξ gives

$$\xi_j(t) = \frac{1}{\omega^2}\sum_k\frac{\partial U}{\partial\bar{q}_k}\frac{\partial^2 H_0}{\partial\bar{p}_k\partial\bar{p}_j}\sin\omega t + \mathcal{O}(\omega^{-3}), \tag{7.15}$$

where the extra accuracy is from integrating only over times of order ω^{-1}. Now the mean values can be evaluated:

$$\begin{aligned}
\langle\eta_k\eta_\ell\rangle &= \frac{1}{2\omega^2}\frac{\partial U}{\partial\bar{q}_k}\frac{\partial U}{\partial\bar{q}_\ell},\\
\langle\xi_k\sin\omega t\rangle &= \frac{1}{2\omega^2}\frac{\partial U}{\partial\bar{q}_k}\frac{\partial^2 H_0}{\partial\bar{p}_k\partial\bar{p}_\ell}.
\end{aligned}$$

Inserting these into the equations of motion (7.12) gives exactly the Hamilton equations which come from the **mean motion Hamiltonian**

$$K(\bar{q},\bar{p}) = H_0(\bar{q},\bar{p}) + \frac{1}{4\omega^2}\sum_{k\ell}\frac{\partial U}{\partial\bar{q}_k}\frac{\partial U}{\partial\bar{q}_\ell}\frac{\partial^2 H_0}{\partial\bar{p}_k\partial\bar{p}_\ell}. \tag{7.16}$$

We see that the mean motion is perturbed only by terms of order $\omega^{-2}\tau^2$, where τ is a typical time for the unperturbed hamiltonian, so the perturbation is small, even though the original perturbing potential is not small at generic instants of time.

The careful reader will be bothered by the contributions of slowly varying terms multiplied by a single η_k or by $\sin\omega t$, for which the average over a period will vanish to order ω^{-1} but not necessarily to order ω^{-2}. Thus the corrections to the motion of $\bar{q}$ and $\bar{p}$ clearly vanish to order ω^{-1}, which is enough to establish the equations for $\vec{\xi}(t)$ and $\vec{\eta}(t)$. But there are still ambiguities of order ω^{-2} in η_k and contributions of that order from $\sin\omega t\vec{\nabla}U$.

The problem arises from the ambiguity in defining the average motions by subtracting off the oscillations. Given the function $p(t)$ with the assurance that its derivative is order 1 as $\omega \to \infty$, we might try to make this subtraction by defining

$$\bar{p}(t) := \frac{\omega}{2\pi}\int_{t-\pi/\omega}^{t+\pi/\omega} p(t')dt',$$

and the rapidly oscillating part $\eta(t) = p(t) - \bar{p}(t)$. But we have not completely eliminated $\langle\eta\rangle$, for over the cycle centered at t,

$$\langle\eta\rangle := \frac{\omega}{2\pi}\int_{t-\pi/\omega}^{t+\pi/\omega}\eta(t')dt' = \bar{p}(t) - \left(\frac{\omega}{2\pi}\right)^2\int_{t-\pi/\omega}^{t+\pi/\omega}dt'\int_{t'-\pi/\omega}^{t'+\pi/\omega}p(t'')dt''.$$

In the last term we interchange orders of integration,

$$\begin{aligned}-\left(\frac{2\pi}{\omega}\right)^2(\langle\eta\rangle - \bar{p}(t)) &= \int_{t-2\pi/\omega}^{t+2\pi/\omega}dt''p(t'')\int_0^{2\pi/\omega-|t''-t|}du \\ &= \int_{t-2\pi/\omega}^{t+2\pi/\omega}dt''p(t'')\left(\frac{2\pi}{\omega}-|t''-t|\right).\end{aligned}$$

So what! If I could assume p had a reasonable power series expansion I could evaluate this, but only the first derivative is known to stay bounded as $\omega \to \infty$. In fact, $\bar{p}$ is probably better defined with a smooth smearing function, say a Gaussian of width $\omega^{-1/2}$ or so.

Another approach would be to relax the zero condition, take the expressions for $\xi(t)$ and $\eta(t)$ to be exact (as they can be considered arbitrary subtractions), and then ask if the $\bar{q}$ and $\bar{p}$ given by H satisfy

the equations given by K solve the original equations through second order. But the answer is no, because there is a term $\propto \cos^2 \omega t$ from the $\eta_k \eta_\ell$ term in 7.8. Perhaps we could add a higher order higher frequency term to η_k?

Let us simplify to one degree of freedom and one parameter, and write

$$\eta(t) = \frac{a_1}{\omega} e^{i\omega t} + \frac{a_2}{\omega^2} e^{2i\omega t}$$
$$\xi(t) = \frac{b_1}{\omega^2} e^{i\omega t} + \frac{b_2}{\omega^3} e^{2i\omega t}$$

so to order ω^{-2} inclusive,

$$\dot\eta = \left(i a_1 + \frac{\dot a_1}{\omega} \right) e^{i\omega t} + \left(\frac{2i a_2}{\omega} + \frac{\dot a_2}{\omega^2} \right) e^{2i\omega t}$$

$$\dot\xi = \left(\frac{i b_1}{\omega} + \frac{\dot b_1}{\omega^2} \right) e^{i\omega t} + \frac{2i b_2}{\omega^2} e^{2i\omega t}$$

The equations of motion are

$$\begin{aligned}
\dot{\bar q} + \dot\xi &= \frac{\partial H_0}{\partial p} + \xi \frac{\partial^2 H_0}{\partial p \partial q} + \eta \frac{\partial^2 H_0}{\partial p \partial p} + \frac{1}{2}\eta^2 \frac{\partial^3 H_0}{\partial p^3} + \mathcal{O}(\omega^{-3}) \\
\dot{\bar p} + \dot\eta &= -\frac{\partial H_0}{\partial q} - \xi \frac{\partial^2 H_0}{\partial q^2} - \eta \frac{\partial^2 H_0}{\partial q \partial p} - \frac{1}{2}\eta^2 \frac{\partial^3 H_0}{\partial q \partial^2 p} - \sin\omega t \frac{\partial U}{\partial q} - \xi \sin\omega t \frac{\partial^2 U}{\partial q^2}
\end{aligned}$$

Assuming all rapidly oscillating terms are in the right place,

$$\begin{aligned}
\left(\frac{i b_1}{\omega} + \frac{\dot b_1}{\omega^2} \right) e^{i\omega t} + \frac{2i b_2}{\omega^2} e^{2i\omega t} = &+ \left(\frac{b_1}{\omega^2} e^{i\omega t} + \frac{b_2}{\omega^3} e^{2i\omega t} \right) \frac{\partial^2 H_0}{\partial p \partial q} \\
&+ \left(\frac{a_1}{\omega} e^{i\omega t} + \frac{a_2}{\omega^2} e^{2i\omega t} \right) \frac{\partial^2 H_0}{\partial p \partial p} + \frac{1}{2} \left(\frac{a_1}{\omega} \right)^2 e^{2i\omega t} \frac{\partial^3 H_0}{\partial p^3}
\end{aligned}$$

$$\begin{aligned}
\left(i a_1 + \frac{\dot a_1}{\omega} \right) e^{i\omega t} + \left(\frac{2i a_2}{\omega} + \frac{\dot a_2}{\omega^2} \right) e^{2i\omega t} = &- \frac{b_1}{\omega^2} e^{i\omega t} \frac{\partial^2 H_0}{\partial q^2} \\
&- \left(\frac{a_1}{\omega} e^{i\omega t} + \frac{a_2}{\omega^2} e^{2i\omega t} \right) \frac{\partial^2 H}{\partial q \partial p} - \frac{1}{2} \left(\frac{a_1}{\omega} \right)^2 e^{2i\omega t} \frac{\partial^3 H}{\partial q \partial^2 p} - \sin\omega t \frac{\partial U}{\partial q} \\
&- \frac{b_1}{\omega^2} e^{i\omega t} \sin\omega t \frac{\partial^2 U}{\partial q^2}
\end{aligned}$$

This seems to say a_2 is order ω^{-1}, so neither η nore ξ do have corrections of order ω^{-2}, although their derivatives do. Let us try another approach,

7.5 New approach

Let

$$\begin{aligned}\xi(t) &= \frac{1}{\omega^2}\frac{\partial U}{\partial q}\frac{\partial^2 H}{\partial p^2}\sin\omega t + \frac{1}{\omega^2}\xi' \\ \eta(t) &= \frac{1}{\omega}\frac{\partial U}{\partial q}\cos\omega t + \frac{1}{\omega^2}\eta'\end{aligned}$$

and assume $\bar{q}$ and $\bar{p}$ obey Hamiltons equations with K.

Then 7.8 says

$$\begin{aligned}&\frac{1}{4\omega^2}\frac{\partial}{\partial p}\left(\left(\frac{\partial U}{\partial q}\right)^2\frac{\partial^2 H}{\partial p^2}\right) + \frac{1}{\omega}\frac{\partial U}{\partial q}\frac{\partial^2 H}{\partial p^2}\cos\omega t + \frac{1}{\omega^2}\sin\omega t\frac{d}{dt}\left(\frac{\partial U}{\partial q}\frac{\partial^2 H}{\partial p^2}\right) + \frac{1}{\omega^2}\dot{\xi}' \\ &\quad= \frac{1}{\omega^2}\sum_k \frac{\partial U}{\partial q}\frac{\partial^2 H}{\partial p^2}\frac{\partial^2 H}{\partial q\partial p}\sin\omega t + \frac{1}{\omega^2}\xi'\frac{\partial^2 H}{\partial q\partial p} + \frac{1}{\omega}\frac{\partial U}{\partial q}\frac{\partial^2 H}{\partial p^2}\cos\omega t \\ &\qquad+\frac{1}{\omega^2}\eta'\frac{\partial^2 H}{\partial p^2} + \frac{1}{2\omega^2}\left(\frac{\partial U}{\partial q}\right)^2\cos^2\omega t\frac{\partial^3 H}{\partial p^3}, \\ &-\frac{1}{4\omega^2}\frac{\partial}{\partial q}\left(\left(\frac{\partial U}{\partial q}\right)^2\frac{\partial^2 H}{\partial p^2}\right) + \frac{1}{\omega}\frac{d}{dt}\left(\frac{\partial U}{\partial q}\right)\cos\omega t - \frac{\partial U}{\partial q}\sin\omega t + \frac{1}{\omega^2}\dot{\eta}' \\ &\quad= -\frac{1}{\omega^2}\frac{\partial U}{\partial q}\frac{\partial^2 H}{\partial p^2}\frac{\partial^2 H}{\partial q^2}\sin\omega t - \frac{1}{\omega^2}\xi'\frac{\partial^2 H}{\partial q^2} - \frac{1}{\omega}\frac{\partial U}{\partial q}\cos\omega t\frac{\partial^2 H}{\partial q\partial p} \\ &\qquad-\frac{1}{\omega^2}\eta'\frac{\partial^2 H}{\partial q\partial p} - \frac{1}{2\omega^2}\left(\frac{\partial U}{\partial q}\right)^2\cos^2\omega t\frac{\partial^3 H}{\partial q\partial p^2} - \frac{\partial U}{\partial q}\sin\omega t \\ &\qquad-\frac{1}{\omega^2}\frac{\partial U}{\partial q}\frac{\partial^2 H}{\partial p^2}\sin^2\omega t\frac{\partial^2 U}{\partial q^2} - \frac{1}{\omega^2}\xi'\sin\omega t\frac{\partial^2 U}{\partial q^2}\end{aligned}$$

Cancel the obvious terms, use $d(\partial U/\partial q)/dt = (\partial^2 U/\partial q^2)(\partial H/\partial p) + \mathcal{O}(\omega^{-2})$, to get

$$\frac{1}{4\omega^2}\left(\frac{\partial U}{\partial q}\right)^2\frac{\partial^3 H}{\partial p^3} + \frac{1}{\omega^2}\sin\omega t\frac{d}{dt}\left(\frac{\partial U}{\partial q}\frac{\partial^2 H}{\partial p^2}\right) + \frac{1}{\omega^2}\dot{\xi}'$$

$$
\begin{aligned}
&= \frac{1}{\omega^2}\sum_k \frac{\partial U}{\partial q}\frac{\partial^2 H}{\partial p^2}\frac{\partial^2 H}{\partial q \partial p}\sin\omega t + \frac{1}{\omega^2}\xi'\frac{\partial^2 H}{\partial q \partial p} \\
&\quad + \frac{1}{\omega^2}\eta'\frac{\partial^2 H}{\partial p^2} + \frac{1}{2\omega^2}\left(\frac{\partial U}{\partial q}\right)^2 \cos^2\omega t \frac{\partial^3 H}{\partial p^3}, \\
&-\frac{1}{2\omega^2}\frac{\partial U}{\partial q}\frac{\partial^2 U}{\partial q^2}\frac{\partial^2 H}{\partial p^2} - \frac{1}{4\omega^2}\left(\frac{\partial U}{\partial q}\right)^2 \frac{\partial^3 H}{\partial q \partial p^2} + \frac{1}{\omega}\frac{\partial^2 U}{\partial q^2}\frac{\partial H}{\partial p}\cos\omega t + \frac{1}{\omega^2}\dot{\eta}' \\
&= -\frac{1}{\omega^2}\frac{\partial U}{\partial q}\frac{\partial^2 H}{\partial p^2}\frac{\partial^2 H}{\partial q^2}\sin\omega t - \frac{1}{\omega^2}\xi'\frac{\partial^2 H}{\partial q^2} - \frac{1}{\omega}\frac{\partial U}{\partial q}\cos\omega t \frac{\partial^2 H}{\partial q \partial p} \\
&\quad - \frac{1}{\omega^2}\eta'\frac{\partial^2 H}{\partial q \partial p} - \frac{1}{2\omega^2}\left(\frac{\partial U}{\partial q}\right)^2 \cos^2\omega t \frac{\partial^3 H}{\partial q \partial p^2} \\
&\quad - \frac{1}{\omega^2}\frac{\partial U}{\partial q}\frac{\partial^2 H}{\partial p^2}\sin^2\omega t \frac{\partial^2 U}{\partial q^2} - \frac{1}{\omega^2}\xi'\sin\omega t \frac{\partial^2 U}{\partial q^2}
\end{aligned}
$$

Now bring the first terms on the left to the other side and use $\cos 2\omega t = 2\cos^2\omega t - 1 = -(2\sin^2\omega t - 1)$, to get

$$
\begin{aligned}
&\frac{1}{\omega^2}\sin\omega t \frac{d}{dt}\left(\frac{\partial U}{\partial q}\frac{\partial^2 H}{\partial p^2}\right) + \frac{1}{\omega^2}\dot{\xi}' \\
&= \frac{1}{\omega^2}\sum_k \frac{\partial U}{\partial q}\frac{\partial^2 H}{\partial p^2}\frac{\partial^2 H}{\partial q \partial p}\sin\omega t + \frac{1}{\omega^2}\xi'\frac{\partial^2 H}{\partial q \partial p} + \frac{1}{\omega^2}\eta'\frac{\partial^2 H}{\partial p^2} \\
&\quad + \frac{1}{4\omega^2}\left(\frac{\partial U}{\partial q}\right)^2 \frac{\partial^3 H}{\partial p^3}\cos 2\omega t, \\
&\frac{1}{\omega^2}\dot{\eta}' = -\frac{1}{\omega^2}\frac{\partial U}{\partial q}\frac{\partial^2 H}{\partial p^2}\frac{\partial^2 H}{\partial q^2}\sin\omega t - \frac{1}{\omega^2}\xi'\frac{\partial^2 H}{\partial q^2} - \frac{1}{\omega}\cos\omega t \frac{\partial}{\partial q}\left(\frac{\partial U}{\partial q}\frac{\partial H}{\partial p}\right) \\
&\quad - \frac{1}{\omega^2}\eta'\frac{\partial^2 H}{\partial q \partial p} - \frac{1}{4\omega^2}\left(\frac{\partial U}{\partial q}\right)^2 \frac{\partial^3 H}{\partial q \partial p^2}\cos 2\omega t \\
&\quad + \frac{1}{2\omega^2}\frac{\partial U}{\partial q}\frac{\partial^2 H}{\partial p^2}\frac{\partial^2 U}{\partial q^2}\cos 2\omega t - \frac{1}{\omega^2}\xi'\sin\omega t \frac{\partial^2 U}{\partial q^2}
\end{aligned}
$$

Note that there is a term of higher order in the $\dot{\eta}'$ expression, so

$$\eta' = \sin\omega t \frac{\partial}{\partial q}\left(\frac{\partial U}{\partial q}\frac{\partial H}{\partial p}\right) + \mathcal{O}(\omega^{-3}).$$

All the other terms are consistent with an $\mathcal{O}(\omega^{-3})$ rapidly oscillating contribution.

Exercises

7.1 Consider the harmonic oscillator $H = p^2/2m + \frac{1}{2}m\omega^2 q^2$ as a perturbation on a free particle $H_0 = p^2/2m$. Find Hamilton's Principle Function $S(q, P)$ which generates the transformation of the unperturbed hamiltonian to Q, P the initial position and momentum. From this, find the Hamiltonian $K(Q, P, t)$ for the full harmonic oscillator, and thus equations of motion for Q and P. Solve these iteratively, assuming $P(0) = 0$, through fourth order in ω. Express q and p to this order, and compare to the exact solution for an harmonic oscillator.

7.2 Consider the Kepler problem in two dimensions. That is, a particle of (reduced) mass μ moves in two dimensions under the influence of a potential

$$U(x, y) = -\frac{K}{\sqrt{x^2 + y^2}}.$$

This is an integrable system, with two integrals of the motion which are in involution. In answering this problem you are expected to make use of the explicit solutions we found for the Kepler problem.
a) What are the two integrals of the motion, F_1 and F_2, in more familiar terms and in terms of explicit functions on phase space.
b) Show that F_1 and F_2 are in involution.
c) Pick an appropriate $\eta_0 \in \mathcal{M}_{\vec{f}}$, and explain how the coordinates $\vec{t}$ are related to the phase space coordinates $\eta = g^{\vec{t}}(\eta_0)$. This discussion may be somewhat qualitative, assuming we both know the explicit solutions of Chapter 3, but it should be clearly stated.
d) Find the vectors $\vec{e}_i$ which describe the unit cell, and give the relation between the angle variables ϕ_i and the usual coordinates η. One of these should be explicit, while the other may be described qualitatively.
e) Comment on whether there are relations among the frequencies and whether this is a degenerate system.

Chapter 8

Field Theory

In section 5.4 we considered the continuum limit of a chain of point masses on stretched string. We had a situation in which the potential energy had interaction terms for particle A which depended only on the relative displacements of particles in the neighborhood of A. If we take our coordinates to be displacements from equilibrium, and consider only motions for which the displacement $\eta = \eta(x, y, z, t)$ becomes differentiable in the continuum limit, then the leading term in the potential energy is proportional to second derivatives in the spacial coordinates. For our points on a string at tension τ, with mass density ρ, we found

$$\begin{aligned} T &= \frac{1}{2}\rho \int_0^L \dot{y}^2(x)dx, \\ U &= \frac{\tau}{2} \int_0^L \left(\frac{\partial y}{\partial x}\right)^2 dx, \end{aligned}$$

as we can write the Lagrangian as an integral of a **Lagrangian density** $\mathcal{L}(y, \dot{y}, y', x, t)$. Actually for our string we had no y or x or t dependence, because we ignored gravity $U_g = \int \rho g y(x, t)dx$, and had a homogeneous string whose properties were time independent. In general, however, such dependence is quite possible. For a three dimensional object, such as the equations for the displacement of the atoms in a crystal, we might have fields $\vec{\eta}$, the three components of the displacement of a particle, as a function of the three coordinates (x, y, z) determining the particle,

as well as time. Thus the generalized coordinates are the functions $\eta_i(x, y, z, t)$, and the Lagrangian density will depend on these, their gradients, their time derivatives, as well as possibly on x, y, z, t. Thus

$$\mathcal{L} = \mathcal{L}(\eta_i, \frac{\partial \eta_i}{\partial x}, \frac{\partial \eta_i}{\partial y}, \frac{\partial \eta_i}{\partial z}, \frac{\partial \eta_i}{\partial t}, x, y, z, t)$$

and

$$\begin{aligned} L &= \int dx\, dy\, dz\, \mathcal{L}, \\ I &= \int dx\, dy\, dz\, dt\, \mathcal{L}. \end{aligned}$$

The actual motion of the system will be given by a particular set of functions $\eta_i(x, y, z, t)$, which are functions over the volume in question and of $t \in [t_I, t_f]$. The function will be determined by the laws of dynamics of the system, together with boundary conditions which depend on the initial configuration $\eta_I(x, y, z, t_I)$ and perhaps a final configuration. Generally there are some boundary conditions on the spacial boundaries as well. For example, our stretched string required $y = 0$ at $x = 0$ and $x = L$.

Before taking the continuum limit we say that the configuration of the system at a given t was a point in a large N dimensional configuration space, and the motion of the system is a path $\Gamma(t)$ in this space. In the continuum limit $N \to \infty$, so we might think of the path as a path in an infinite dimensional space. But we can also think of this path as a mapping $t \to \eta(\cdot, \cdot, \cdot, t)$ of time into the (infinite dimensional) space of functions on ordinary space.

Hamilton's principal says that the actual path is an extremum of the action. If we consider small variations $\delta\eta_i(x, y, z, t)$ which vanish on the boundaries, then

$$\delta I = \int dx\, dy\, dz\, dt\, \delta\mathcal{L} = 0.$$

Note that what is varied here are the functions η_i, not the coordinates (x, y, z, t). x, y, z do not represent the position of some atom — they represent a label which tells us which atom it is that we are talking about. They may well be the equilibrium position of that atom, but

they are independent of the motion. It is the η_i which are the dynamical degrees of freedom, specifying the configuration of the system.

The variation

$$\begin{aligned}\delta\mathcal{L}(\eta_i, \frac{\partial\eta_i}{\partial x}, \frac{\partial\eta_i}{\partial y}, \frac{\partial\eta_i}{\partial z}, \frac{\partial\eta_i}{\partial t}, x, y, z, t)\\ = \frac{\partial\mathcal{L}}{\partial\eta}\delta\eta + \frac{\partial\mathcal{L}}{\partial(\partial\eta/\partial x)}\delta\frac{\partial\eta}{\partial x} + \frac{\partial\mathcal{L}}{\partial(\partial\eta/\partial y)}\delta\frac{\partial\eta}{\partial y} + \frac{\partial\mathcal{L}}{\partial(\partial\eta/\partial z)}\delta\frac{\partial\eta}{\partial z}\\ + \frac{\partial\mathcal{L}}{\partial(\partial\eta/\partial t)}\delta\frac{\partial\eta}{\partial t}.\end{aligned}$$

Notice there is no variation of x, y, z, and t, as we discussed.

The notation is getting awkward, so we need to reintroduce the notation $A_{,i} = \partial A/\partial r_i$. In fact, we see that $\partial/\partial t$ enters in the same way as $\partial/\partial x$, so we will set $x_0 = t$ and write

$$\partial_\mu := \frac{\partial}{\partial x_\mu} = \left(\frac{\partial}{\partial t}, \frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z}\right),$$

for $\mu = 0, 1, 2, 3$, and write $\eta_{,\mu} := \partial_\mu\eta$. If there are several fields η_i, then $\partial_\mu\eta_i = \eta_{i,\mu}$. The comma represents the beginning of differentiation, so we must not use one to separate different ordinary indices.

In this notation, we have

$$\delta\mathcal{L} = \sum_i \frac{\partial\mathcal{L}}{\partial\eta_i}\delta\eta_i + \sum_i\sum_{\mu=0}^{3}\frac{\partial\mathcal{L}}{\partial\eta_{i,\mu}}\delta\eta_{i,\mu},$$

and

$$\delta I = \int\left(\sum_i \frac{\partial\mathcal{L}}{\partial\eta_i}\delta\eta_i + \sum_i\sum_{\mu=0}^{3}\frac{\partial\mathcal{L}}{\partial\eta_{i,\mu}}\delta\eta_{i,\mu}\right)d^4x,$$

where $d^4x = dx\,dy\,dz\,dt$. Except for the first term, we integrate by parts,

$$\delta I = \int\left[\sum_i \frac{\partial\mathcal{L}}{\partial\eta_i} - \sum_i\sum_{\mu=0}^{3}\left(\partial_\mu\frac{\partial\mathcal{L}}{\partial\eta_{i,\mu}}\right)\right]\delta\eta_i d^4x,$$

where we have thrown away the boundary terms which involve $\delta\eta_i$ evaluated on the boundary, which we assumed to be zero. Inside the region of integration, the $\delta\eta_i$ are independent, so requiring $\delta I = 0$ for all functions $\delta\eta_i(x_\mu)$ implies

$$\partial_\mu \frac{\partial \mathcal{L}}{\partial \eta_{i,\mu}} - \frac{\partial \mathcal{L}}{\partial \eta_i} = 0. \tag{8.1}$$

We have written the equations of motion (which is now a partial differential equation rather than coupled ordinary differential equations), in a form which looks like we are dealing with a relativistic problem, because t and spatial coordinates are entering in the same way. We have not made any assumption of relativity, however, and our problem will not be relativistically invariant unless the Lagrangian density is invariant under Lorentz transformations (as well as translations).

Now consider how the Lagrangian changes from one point in spacetime to another, including the variation of the fields, assuming the fields obey the equations of motion. Then the total derivative for a variation of x_μ is

$$\frac{d\mathcal{L}}{dx_\mu} = \left.\frac{\partial \mathcal{L}}{\partial x_\mu}\right|_\eta + \frac{\partial \mathcal{L}}{\partial \eta_i}\eta_{i,\mu} + \frac{\partial \mathcal{L}}{\partial \eta_{i,\nu}}\eta_{i,\nu,\mu}.$$

Plugging the equations of motion into the second term,

$$\begin{aligned} \frac{d\mathcal{L}}{dx_\mu} &= \frac{\partial \mathcal{L}}{\partial x_\mu} + \partial_\nu\left(\frac{\partial \mathcal{L}}{\partial \eta_{i,\nu}}\right)\eta_{i,\mu} + \frac{\partial \mathcal{L}}{\partial \eta_{i,\nu}}\eta_{i,\mu,\nu} \\ &= \frac{\partial \mathcal{L}}{\partial x_\mu} + \partial_\nu\left(\frac{\partial \mathcal{L}}{\partial \eta_{i,\nu}}\eta_{i,\mu}\right). \end{aligned}$$

Thus

$$\partial_\nu T_{\mu\nu} = -\frac{\partial \mathcal{L}}{\partial x_\mu}, \tag{8.2}$$

where the **stress-energy** tensor $T_{\mu\nu}$ is defined by

$$T_{\mu\nu}(x) = \frac{\partial \mathcal{L}}{\partial \eta_{i,\nu}}\eta_{i,\mu} - \mathcal{L}\delta_{\mu\nu}. \tag{8.3}$$

Note that if the Lagrangian density has no *explicit* dependence on the coordinates x_μ, the stress-energy tensor satisfies an equation $\partial_\nu T_{\mu\nu}$ which is a continuity equation.

In dynamics of discrete systems we defined the Hamiltonian as $H = \sum_i p_i \dot{q}_i - L(q,p,t)$. Considering the continuum as a limit, $L = \int d^3x \mathcal{L}$ is the limit of $\sum_{ijk} \Delta x \Delta y \Delta z L_{ijk}$, where L_{ijk} depends on q_{ijk} and a few of its neighbors, and also on $\dot{q}_{ijk}$. The conjugate momentum $p_{ijk} = \partial L/\partial \dot{q}_{ijk} = \Delta x \Delta y \Delta z \partial L_{ijk}/\partial \dot{q}_{ijk}$ which would vanish in the continuum limit, so instead we define

$$\pi(x,y,z) = p_{ijk}/\Delta x \Delta y \Delta z = \partial L_{ijk}/\partial \dot{q}_{ijk} = \delta \mathcal{L}/\delta \dot{q}(x,y,z).$$

The Hamiltonian

$$\begin{aligned} H &= \sum p_{ijk}\dot{q}_{ijk} - L = \sum \Delta x \Delta y \Delta z \pi(x,y,z)\dot{q}(xyz) - L \\ &= \int d^3x \left(\pi(\vec{r})\dot{q}(\vec{r}) - \mathcal{L}\right) = \int d^3x \mathcal{H}, \end{aligned}$$

where the **Hamiltonian density** is defined by

$$\mathcal{H}(\vec{r}) = \pi(\vec{r})\dot{q}(\vec{r}) - \mathcal{L}(\vec{r}).$$

Of course if there are several fields q_i at each point,

$$\mathcal{H}(\vec{r}) = \sum_i \pi_i(\vec{r})\dot{q}_i(\vec{r}) - \mathcal{L}(\vec{r}).$$

where

$$\pi_i(\vec{r}) = \frac{\delta \mathcal{L}}{\delta \dot{q}_i(\vec{r})}.$$

Notice that the Hamiltonian density is exactly T_{00}, one component of the stress-energy tensor.

Consider the case where $\mathcal{L}$ does not depend explicitly on $(\vec{x},t)$, so

$$\sum_{\nu=0}^{3} \partial_\nu T_{\mu\nu} = 0,$$

or

$$\frac{\partial}{\partial t} T_{\mu 0} = \sum_{i=1}^{3} \partial_i T_{\mu i} = 0.$$

This is a continuity equation, similar to the equation from fluid mechanics, $\partial\rho/\partial t + \vec{\nabla}\cdot(\rho\vec{v}) = 0$, which expresses the conservation of mass. That equation has the interpretation that the change in the mass contained in some volume is equal to the flux into the volume, because $\rho\vec{v}$ is the flow of mass past a unit surface area. In the current case, we have four conservation equations, indexed by μ. Each of these can be integrated over space to tell us about the rate of change of the "charge" $Q_\mu(t) = \int d^3V\, T_{\mu 0}(\vec{x},t)$,

$$\frac{d}{dt}Q_\mu(t) = \int d^3V\, \frac{\partial}{\partial x_i}T_{\mu i}(\vec{x},t).$$

We see that his is the integral of the divergence of a vector current $(\vec{J}_\mu)_i = T_{\mu i}$, which by Gauss' law becomes a surface integral of the flux of J_μ out of the volume of our system. We have been sloppy about our boundary conditions, but in many cases it is reasonable to assume there is no flux out of the volume. In this case the right hand side vanishes, and we find four conserved quantities

$$Q_\mu(t) = \text{constant}.$$

For $\mu = 0$ we saw that T_{00} is the energy density, so Q_0 is the total energy.

Cyclic coordinates

In discrete mechanics, when L was independent of a coordinate q_i, even though it depended on $\dot{q}_i$, we called the coordinate cyclic or ignorable, and found a conserved momentum conjugate to it. For fields in general, $\mathcal{L}(\eta,\dot{\eta},\nabla\eta)$ depends on spatial derivates of η as well, and we may ask whether we need to require absense of dependence on $\nabla\eta$ for a coordinate to be cyclic. Independence of both η and $\nabla\eta$ implies independence on an infinite number of discrete coordinates, the values of $\eta(\vec{r})$ at every point $\vec{r}$, which is too restrictive a condition for our discussion. We will call a coordinate field η_i cyclic if $\mathcal{L}$ does not depend directly on η_i, although it may depend on its derivatives $\dot{\eta}_i$ and $\nabla\eta_i$.

The Lagrange equation then states

$$\sum_\mu \partial_\mu \frac{\delta\mathcal{L}}{\delta\eta_{i,\mu}} = 0, \quad \text{or } \frac{d}{dt}\pi_i + \sum_j \partial_j \frac{\delta\mathcal{L}}{\delta\eta_{i,j}} = 0.$$

If we integrate this equation over all space, and define

$$\Pi_i(t) = \int \pi_i(\vec{r}) d^3r,$$

then the derivative $d\Pi/dt$ involves the integral of a divergence, which by Gauss' law is a surface term

$$\frac{d\Pi(t)}{dt} = -\int \frac{\delta \mathcal{L}}{\delta \eta_{i,j}} (dS)_j.$$

Assuming the spatial boundary conditions are such that we may ignore this boundary term, we see that $\Pi_i(t)$ is a constant of the motion.

8.1 Noether's Theorem

We want to discuss the relationship between symmetries and conserved quantities which is known as **Noether's theorem**. It concerns infinitesimal tranformations of the degrees of freedom $\eta_i(x_\mu)$ which may relate these to degrees of freedom at a changed point. That is, the new fields $\eta'(x')$ is related to $\eta(x)$ rather than $\eta(x')$, where $x_\mu \to x'_\mu = x_\mu + \delta x_\mu$ is some infinitesimal transformation of the coordinates rather than of the degrees of freedom. For a scalar field, like temperature, under a rotation, we would define the new field

$$\eta'(x') = \eta(x),$$

but more generally the field may also change, in a way that may depend on other fields,

$$\eta'_i(x') = \eta_i(x) + \delta\eta_i(x; \eta_k(x)).$$

This is what you would expect for a vector field $\vec{E}$ under rotations, because the new E'_x gets a component from the old E_y.

The Lagrangian is a given function of the old fields $\mathcal{L}(\eta_i, \eta_{i,\mu}, x_\mu)$. If we substitute in the values of $\eta(x)$ in terms of $\eta'(x')$ we get a new function $\mathcal{L}'$, defined by

$$\mathcal{L}'(\eta'_i, \eta'_{i,\mu}, x'_\mu) = \mathcal{L}(\eta_i, \eta_{i,\mu}, x_\mu).$$

The symmetries we wish to discuss are transformations of this type under which the form of the Lagrangian density does not change, so that $\mathcal{L}'$ is the same functional form as $\mathcal{L}$, or

$$\mathcal{L}'(\eta_i', \eta_{i,\mu}', x_\mu') = \mathcal{L}(\eta_i', \eta_{i,\mu}', x_\mu').$$

In considering the action, we integrate the Lagrangian density over a region of space-time between two spacial slices corresponding to an initial time and a final time. We may, however, consider an arbitrary region of spacetime $\Omega \subset \mathbb{R}^4$. The corresponding four dimensional volume in the transformed coordinates is the region $x' \in \Omega'$. The action for a given field configuration η

$$S(\eta) = \int_\Omega \mathcal{L}(\eta, \eta_{,\mu}, x) d^4x$$

differs from $S'(\eta') = \int_{\Omega'} \mathcal{L}'(\eta', \eta_{,\mu}', x') d^4x')$ only by the Jacobian, as a change of variables gives

$$S'(\eta') = \int_\Omega \left| \frac{\partial x'}{\partial x} \right| \mathcal{L}(\eta, \eta_{,\mu}, x) d^4x.$$

The Jacobian is

$$\det\left(\delta_{\mu\nu} + \partial_\nu \delta x_\mu\right) = 1 + \operatorname{Tr} \frac{\partial \delta x_\mu}{\partial x_\nu} = 1 + \partial_\mu \delta x_\mu.$$

It makes little sense to assume the Lagrangian *density* is invariant unless the volume element is as well, so we will require the Jacobian to be identically 1, or $\partial_\mu \delta x_\mu = 0$. So then $\delta S = 0$ for the symmetries we wish to discuss.

We can also consider $S'(x')$ as an integral over x, as this is just a dummy variable,

$$S'(\eta') = \int_{\Omega'} \mathcal{L}\left(\eta'(x), \eta_{,\mu}'(x), x\right) d^4x.$$

This differs from $S(\eta)$ by $S'(\eta') - S(\eta) = \delta_1 S + \delta_2 S$, because

1. the Lagrangian is evaluated with the field η' rather than η, producing a change

$$\delta_1 S = \int \left(\frac{\delta \mathcal{L}}{\delta \eta_i} \bar{\delta} \eta_i + \frac{\delta \mathcal{L}}{\delta \eta_{i,\mu}} \bar{\delta} \eta_{i,\mu} \right) d^4x,$$

where

$$\bar{\delta}\eta_i(x) := \eta_i'(x) - \eta_i(x) = \eta_i'(x) - \eta_i'(x') + \delta\eta_i(x) = \delta\eta_i(x) - \eta_{i,\mu}\delta x_\mu.$$

2. Change in the region of integration, Ω' rather than Ω,

$$\delta_2 S = \left(\int_{\Omega'} - \int_{\Omega}\right) \mathcal{L}(\eta, \eta_{,\mu}, x) d^4x.$$

If we define $d\Sigma_\mu$ to be an element of the three dimensional surface $\Sigma = \partial\Omega$ of Ω, with outward-pointing normal in the direction of $d\Sigma_\mu$, the difference in the regions of integration may be written as an integral over the surface,

$$\left(\int_{\Omega'} - \int_{\Omega}\right) d^4x = \int_{\Sigma} \delta x_\mu \cdot d\Sigma_\mu.$$

Thus

$$\delta_2 S = \int_{\partial\Omega} \mathcal{L}\delta x_\mu \cdot dS_\mu = \int_{\Omega} \partial_\mu \left(\mathcal{L}\delta x_\mu\right) \tag{8.4}$$

by Gauss' Law (in four dimensions).

As $\bar{\delta}$ is a difference of two functions at the same values of x, this operator commutes with partial differentiation, so $\bar{\delta}\eta_{i,\mu} = \partial_\mu \bar{\delta}\eta_i$. Using this in the second term of $\delta_1 S$ and the equations of motion in the first, we have

$$\begin{aligned}
\delta_1 S &= \int d^4x \left[\left(\partial_\mu \frac{\partial \mathcal{L}}{\partial \eta_{i,\mu}}\right)\bar{\delta}\eta_i + \frac{\partial \mathcal{L}}{\partial \eta_{i,\mu}}\partial_\mu \bar{\delta}\eta_i\right] \\
&= \int_{\Omega} d^4x \partial_\mu \left(\frac{\partial \mathcal{L}}{\partial \eta_{i,\mu}}\bar{\delta}\eta_i\right) \\
&= \int_{\Omega} d^4x \partial_\mu \left(\frac{\partial \mathcal{L}}{\partial \eta_{i,\mu}}\delta\eta_i - \frac{\partial \mathcal{L}}{\partial \eta_{i,\mu}}\eta_{i,\nu}\delta x_\nu\right).
\end{aligned}$$

Then $\delta_1 S + \delta_2 S = 0$ is a condition in the form

$$\int_{\Omega} d^4x \, \partial_\mu J_\mu = 0, \tag{8.5}$$

which holds for arbitrary volumes Ω. Thus we have a conservation equation

$$\partial_\mu J_\mu = 0.$$

The infinitesimal variations may be thought of as proportional to an infinitesimal parameter ϵ, which is often in fact a component of a four-vector. The variations in x_μ and η_i are then

$$\delta x_\mu = \epsilon \frac{dx_\mu}{d\epsilon}, \qquad \delta\eta_i = \epsilon \frac{d\eta_i}{d\epsilon},$$

so if $\delta_1 S + \delta_2 S = 0$ is $-\epsilon$ times (8.5),

$$\begin{aligned} J_\mu &= -\frac{\partial \mathcal{L}}{\partial \eta_{i,\mu}} \frac{d\eta_i}{d\epsilon} + \frac{\partial \mathcal{L}}{\partial \eta_{i,\mu}} \eta_{i,\nu} \frac{dx_\nu}{d\epsilon} - \mathcal{L} \frac{dx_\mu}{d\epsilon}. \\ &= -\frac{\partial \mathcal{L}}{\partial \eta_{i,\mu}} \frac{d\eta_i}{d\epsilon} + T_{\nu\mu} \frac{dx_\nu}{d\epsilon}. \end{aligned} \tag{8.6}$$

Exercises

8.1 The Lagrangian density for the electromagnetic field in vacuum may be written

$$\mathcal{L} = \frac{1}{2}\left(\vec{E}^{\,2} - \vec{B}^{\,2}\right),$$

where the dynamical degrees of freedom are not $\vec{E}$ and $\vec{B}$, but rather $\vec{A}$ and ϕ, where

$$\begin{aligned} \vec{B} &= \vec{\nabla} \times A \\ \vec{E} &= -\vec{\nabla}\phi - \frac{1}{c}\dot{\vec{A}} \end{aligned}$$

a) Find the canonical momenta, and comment on what seems unusual about one of the answers.
b) Find the Lagrange Equations for the system. Relate to known equations for the electromagnetic field.

Appendix A

ϵ_{ijk} and cross products

A.1 Vector Operations

A.1.1 δ_{ij} and ϵ_{ijk}

These are some notes on the use of the antisymmetric symbol ϵ_{ijk} for expressing cross products. This is an extremely powerful tool for manipulating cross products and their generalizations in higher dimensions, and although many low level courses avoid the use of ϵ, I think this is a mistake and I want you to become proficient with it.

In a cartesian coordinate system a vector $\vec{V}$ has components V_i along each of the three orthonormal basis vectors $\hat{e}_i$, or $\vec{V} = \sum_i V_i \hat{e}_i$. The dot product of two vectors, $\vec{A} \cdot \vec{B}$, is bilinear and can therefore be written as

$$\begin{aligned} \vec{A} \cdot \vec{B} &= (\sum_i A_i \hat{e}_i) \cdot \sum_j B_j \hat{e}_j && \text{(A.1)} \\ &= \sum_i \sum_j A_i B_j \hat{e}_i \cdot \hat{e}_j && \text{(A.2)} \\ &= \sum_i \sum_j A_i B_j \delta_{ij}, && \text{(A.3)} \end{aligned}$$

where the Kronecker delta δ_{ij} is defined to be 1 if $i = j$ and 0 otherwise. As the basis vectors $\hat{e}_k$ are orthonormal, *i.e.* orthogonal to each other and of unit length, we have $\hat{e}_i \cdot \hat{e}_j = \delta_{ij}$.

Doing a sum over an index j of an expression involving a δ_{ij} is very simple, because the only term in the sum which contributes is the one with $j = i$. Thus $\sum_j F(i,j)\delta_{ij} = F(i,i)$, which is to say, one just replaces j with i in all the other factors, and drops the δ_{ij} and the summation over j. So we have $\vec{A}\cdot\vec{B} = \sum_i A_i B_i$, the standard expression for the dot product[1]

We now consider the cross product of two vectors, $\vec{A} \times \vec{B}$, which is also a bilinear expression, so we must have $\vec{A} \times \vec{B} = (\sum_i A_i \hat{e}_i) \times (\sum_j B_j \hat{e}_j) = \sum_i \sum_j A_i B_j (\hat{e}_i \times \hat{e}_j)$. The cross product $\hat{e}_i \times \hat{e}_j$ is a vector, which can therefore be written as $\vec{V} = \sum_k V_k \hat{e}_k$. But the vector result depends also on the two input vectors, so the coefficients V_k really depend on i and j as well. Define them to be ϵ_{ijk}, so

$$\hat{e}_i \times \hat{e}_j = \sum_k \epsilon_{kij} \hat{e}_k.$$

It is easy to evaluate the 27 coefficients ϵ_{kij}, because the cross product of two orthogonal unit vectors is a unit vector orthogonal to both of them. Thus $\hat{e}_1 \times \hat{e}_2 = \hat{e}_3$, so $\epsilon_{312} = 1$ and $\epsilon_{k12} = 0$ if $k = 1$ or 2. Applying the same argument to $\hat{e}_2 \times \hat{e}_3$ and $\hat{e}_3 \times \hat{e}_1$, and using the antisymmetry of the cross product, $\vec{A} \times \vec{B} = -\vec{B} \times \vec{A}$, we see that

$$\epsilon_{123} = \epsilon_{231} = \epsilon_{312} = 1; \qquad \epsilon_{132} = \epsilon_{213} = \epsilon_{321} = -1,$$

and $\epsilon_{ijk} = 0$ for all other values of the indices, *i.e.* $\epsilon_{ijk} = 0$ whenever any two of the indices are equal. Note that ϵ changes sign not only when the last two indices are interchanged (a consequence of the antisymmetry of the cross product), but whenever *any* two of its indices are interchanged. Thus ϵ_{ijk} is zero unless $(1,2,3) \to (i,j,k)$ is a permutation, and is equal to the sign of the permutation if it exists.

Now that we have an expression for $\hat{e}_i \times \hat{e}_j$, we can evaluate

$$\vec{A} \times \vec{B} = \sum_i \sum_j A_i B_j (\hat{e}_i \times \hat{e}_j) = \sum_i \sum_j \sum_k \epsilon_{kij} A_i B_j \hat{e}_k. \tag{A.4}$$

Much of the usefulness of expressing cross products in terms of ϵ's comes from the identity

$$\sum_k \epsilon_{kij} \epsilon_{k\ell m} = \delta_{i\ell}\delta_{jm} - \delta_{im}\delta_{j\ell}, \tag{A.5}$$

[1]Note that this only holds because we have expressed our vectors in terms of *orthonormal* basis vectors.

which can be shown as follows. To get a contribution to the sum, k must be different from the unequal indices i and j, and also different from ℓ and m. Thus we get 0 unless the pair (i,j) and the pair (ℓ,m) are the same pair of different indices. There are only two ways that can happen, as given by the two terms, and we only need to verify the coefficients. If $i=\ell$ and $j=m$, the two ϵ's are equal and the square is 1, so the first term has the proper coefficient of 1. The second term differs by one transposition of two indices on one epsilon, so it must have the opposite sign.

We now turn to some applications. Let us first evaluate

$$\vec{A}\cdot(\vec{B}\times\vec{C}) = \sum_i A_i \sum_{jk} \epsilon_{ijk} B_j C_k = \sum_{ijk} \epsilon_{ijk} A_i B_j C_k. \tag{A.6}$$

Note that $\vec{A}\cdot(\vec{B}\times\vec{C})$ is, up to sign, the volume of the parallelopiped formed by the vectors $\vec{A}$, $\vec{B}$, and $\vec{C}$. From the fact that the ϵ changes sign under transpositions of any two indices, we see that the same is true for transposing the vectors, so that

$$\begin{aligned}\vec{A}\cdot(\vec{B}\times\vec{C}) = -\vec{A}\cdot(\vec{C}\times\vec{B}) &= \vec{B}\cdot(\vec{C}\times\vec{A}) = -\vec{B}\cdot(\vec{A}\times\vec{C}) \\ &= \vec{C}\cdot(\vec{A}\times\vec{B}) = -\vec{C}\cdot(\vec{B}\times\vec{A}).\end{aligned}$$

Now consider $\vec{V} = \vec{A}\times(\vec{B}\times\vec{C})$. Using our formulas,

$$\vec{V} = \sum_{ijk} \epsilon_{kij}\hat{e}_k A_i (\vec{B}\times\vec{C})_j = \sum_{ijk} \epsilon_{kij}\hat{e}_k A_i \sum_{lm} \epsilon_{jlm} B_l C_m.$$

Notice that the sum on j involves only the two epsilons, and we can use

$$\sum_j \epsilon_{kij}\epsilon_{jlm} = \sum_j \epsilon_{jki}\epsilon_{jlm} = \delta_{kl}\delta_{im} - \delta_{km}\delta_{il}.$$

Thus

$$\begin{aligned}V_k &= \sum_{ilm}(\sum_j \epsilon_{kij}\epsilon_{jlm}) A_i B_l C_m = \sum_{ilm}(\delta_{kl}\delta_{im} - \delta_{km}\delta_{il}) A_i B_l C_m \\ &= \sum_{ilm} \delta_{kl}\delta_{im} A_i B_l C_m - \sum_{ilm} \delta_{km}\delta_{il} A_i B_l C_m \\ &= \sum_i A_i B_k C_i - \sum_i A_i B_i C_k = \vec{A}\cdot\vec{C}\, B_k - \vec{A}\cdot\vec{B}\, C_k,\end{aligned}$$

so

$$\vec{A} \times (\vec{B} \times \vec{C}) = \vec{B}\, \vec{A} \cdot \vec{C} - \vec{C}\, \vec{A} \cdot \vec{B}. \tag{A.7}$$

This is sometimes known as the **bac-cab** formula.

Exercise: Using (A.5) for the manipulation of cross products, show that

$$(\vec{A} \times \vec{B}) \cdot (\vec{C} \times \vec{D}) = \vec{A} \cdot \vec{C}\vec{B} \cdot \vec{D} - \vec{A} \cdot \vec{D}\vec{B} \cdot \vec{C}.$$

The determinant of a matrix can be defined using the ϵ symbol. For a 3×3 matrix A,

$$\det A = \sum_{ijk} \epsilon_{ijk} A_{1i} A_{2j} A_{3k} = \sum_{ijk} \epsilon_{ijk} A_{i1} A_{j2} A_{k3}.$$

From the second definition, we see that the determinant is the volume of the parallelopiped formed from the images under the linear map A of the three unit vectors $\hat{e}_i$, as

$$(A\hat{e}_1) \cdot ((A\hat{e}_2) \times (A\hat{e}_3)) = \det A.$$

In higher dimensions, the cross product is not a vector, but there is a generalization of ϵ which remains very useful. In an n-dimensional space, $\epsilon_{i_1 i_2 \ldots i_n}$ has n indices and is defined as the sign of the permutation $(1, 2, \ldots, n) \to (i_1 i_2 \ldots i_n)$, if the indices are all unequal, and zero otherwise. The analog of (A.5) has $(n-1)!$ terms from all the permutations of the unsummed indices on the second ϵ. The determinant of an $n \times n$ matrix is defined as

$$\det A = \sum_{i_1, \ldots, i_n} \epsilon_{i_1 i_2 \ldots i_n} \prod_{p=1}^{n} A_{p, i_p}.$$

Appendix B

The gradient operator

We can define the gradient operator

$$\vec{\nabla} = \sum_i \hat{e}_i \frac{\partial}{\partial x_i}. \tag{B.1}$$

While this looks like an ordinary vector, the coefficients are not numbers V_i but are operators, which do not commute with functions of the coordinates x_i. We can still write out the components straightforwardly, but we must be careful to keep the order of the operators and the fields correct.

The gradient of a scalar field $\Phi(\vec{r})$ is simply evaluated by distributing the gradient operator

$$\vec{\nabla}\Phi = (\sum_i \hat{e}_i \frac{\partial}{\partial x_i})\Phi(\vec{r}) = \sum_i \hat{e}_i \frac{\partial \Phi}{\partial x_i}. \tag{B.2}$$

Because the individual components obey the Leibnitz rule $\frac{\partial AB}{\partial x_i} = \frac{\partial A}{\partial x_i}B + A\frac{\partial B}{\partial x_i}$, so does the gradient, so if A and B are scalar fields,

$$\vec{\nabla}AB = (\vec{\nabla}A)B + A\vec{\nabla}B. \tag{B.3}$$

The general application of the gradient operator $\vec{\nabla}$ to a *vector* $\vec{A}$ gives an object with coefficients with two indices, a *tensor*. Some parts of this tensor, however, can be simplified. The first (which is the trace

of the tensor) is called the *divergence* of the vector, written and defined by

$$\begin{aligned}\vec{\nabla}\cdot\vec{A} &= (\sum_i \hat{e}_i\frac{\partial}{\partial x_i})\cdot(\sum_j \hat{e}_j B_j) = \sum_{ij}\hat{e}_i\cdot\hat{e}_j\frac{\partial B_j}{\partial x_i} = \sum_{ij}\delta_{ij}\frac{\partial B_j}{\partial x_i} \\ &= \sum_i \frac{\partial B_i}{\partial x_i}. \end{aligned} \tag{B.4}$$

In asking about Leibnitz' rule, we must remember to apply the divergence operator only to vectors. One possibility is to apply it to the vector $\vec{V} = \Phi\vec{A}$, with components $V_i = \Phi A_i$. Thus

$$\begin{aligned}\vec{\nabla}\cdot(\Phi\vec{A}) &= \sum_i \frac{\partial(\Phi A_i)}{\partial x_i} = \sum_i \frac{\partial\Phi}{\partial x_i}A_i + \Phi\sum_i\frac{\partial A_i}{\partial x_i} \\ &= (\vec{\nabla}\Phi)\cdot\vec{A} + \Phi\vec{\nabla}\cdot\vec{A}. \end{aligned} \tag{B.5}$$

We could also apply the divergence to the cross product of two vectors,

$$\begin{aligned}\vec{\nabla}\cdot(\vec{A}\times\vec{B}) &= \sum_i \frac{\partial(\vec{A}\times\vec{B})_i}{\partial x_i} = \sum_i \frac{\partial(\sum_{jk}\epsilon_{ijk}A_jB_k)}{\partial x_i} = \sum_{ijk}\epsilon_{ijk}\frac{\partial(A_jB_k)}{\partial x_i} \\ &= \sum_{ijk}\epsilon_{ijk}\frac{\partial A_j}{\partial x_i}B_k + \sum_{ijk}\epsilon_{ijk}A_j\frac{\partial B_k}{\partial x_i}. \end{aligned} \tag{B.6}$$

This is expressible in terms of the *curls* of $\vec{A}$ and $\vec{B}$.

The curl is like a cross product with the first vector replaced by the differential operator, so we may write the i'th component as

$$(\vec{\nabla}\times\vec{A})_i = \sum_{jk}\epsilon_{ijk}\frac{\partial}{\partial x_j}A_k. \tag{B.7}$$

We see that the last expression in (B.6) is

$$\sum_k(\sum_{ij}\epsilon_{kij}\frac{\partial A_j}{\partial x_i})B_k - \sum_j A_j\sum_{ik}\epsilon_{jik}\frac{\partial B_k}{\partial x_i} = (\vec{\nabla}\times\vec{A})\cdot\vec{B} - \vec{A}\cdot(\vec{\nabla}\times\vec{B}). \tag{B.8}$$

where the sign which changed did so due to the transpositions in the indices on the ϵ, which we have done in order to put things in the form of the definition of the curl. Thus

$$\vec{\nabla}\cdot(\vec{A}\times\vec{B}) = (\vec{\nabla}\times\vec{A})\cdot\vec{B} - \vec{A}\cdot(\vec{\nabla}\times\vec{B}). \tag{B.9}$$

Vector algebra identities apply to the curl as to any ordinary vector, except that one must be careful not to change, by reordering, what the differential operators act on. In particular, Eq. A.7 is

$$\vec{A} \times (\vec{\nabla} \times \vec{B}) = \sum_i A_i \vec{\nabla} B_i - \sum_i A_i \frac{\partial \vec{B}}{\partial x_i}. \tag{B.10}$$

Appendix C

Gradient in Spherical Coordinates

The transformation between Cartesian and spherical coordinates is given by

$$\begin{array}{ll} r = (x^2+y^2+z^2)^{\frac{1}{2}} & x = r\sin\theta\cos\phi \\ \theta = \cos^{-1}(z/r) & y = r\sin\theta\sin\phi \\ \phi = \tan^{-1}(y/x) & z = r\cos\theta \end{array}$$

The basis vectors $\{\hat{e}_r, \hat{e}_\theta, \hat{e}_\phi\}$ at the point (r, θ, ϕ) are given in terms of the cartesian basis vectors by

$$\begin{aligned} \hat{e}_r &= \sin\theta\cos\phi\,\hat{e}_x + \sin\theta\sin\phi\,\hat{e}_y + \cos\theta\,\hat{e}_z \\ \hat{e}_\theta &= \cos\theta\cos\phi\,\hat{e}_x + \cos\theta\sin\phi\,\hat{e}_y - \sin\theta\,\hat{e}_z \\ \hat{e}_\phi &= -\sin\phi\,\hat{e}_x + \cos\phi\,\hat{e}_y. \end{aligned}$$

By the chain rule, if we have two sets of coordinates, say s_i and c_i, and we know the form a function $f(s_i)$ and the dependence of s_i on c_j, we can find $\frac{\partial f}{\partial c_i} = \sum_j \frac{\partial f}{\partial s_j}\Big|_s \frac{\partial s_j}{\partial c_i}\Big|_c$, where $|_s$ means hold the other s's fixed while varying s_j. In our case, the s_j are the spherical coordinates r, θ, ϕ, while the c_i are x, y, z.

Thus

$$\vec{\nabla} f = \left(\frac{\partial f}{\partial r}\bigg|_{\theta\phi} \frac{\partial r}{\partial x}\bigg|_{yz} + \frac{\partial f}{\partial \theta}\bigg|_{r\phi} \frac{\partial \theta}{\partial x}\bigg|_{yz} + \frac{\partial f}{\partial \phi}\bigg|_{r\theta} \frac{\partial \phi}{\partial x}\bigg|_{yz} \right) \hat{e}_x$$

$$+\left(\left.\frac{\partial f}{\partial r}\right|_{\theta\phi}\left.\frac{\partial r}{\partial y}\right|_{xz}+\left.\frac{\partial f}{\partial \theta}\right|_{r\phi}\left.\frac{\partial \theta}{\partial y}\right|_{xz}+\left.\frac{\partial f}{\partial \phi}\right|_{r\theta}\left.\frac{\partial \phi}{\partial y}\right|_{xz}\right)\hat{e}_y \quad \text{(C.1)}$$

$$+\left(\left.\frac{\partial f}{\partial r}\right|_{\theta\phi}\left.\frac{\partial r}{\partial z}\right|_{xy}+\left.\frac{\partial f}{\partial \theta}\right|_{r\phi}\left.\frac{\partial \theta}{\partial z}\right|_{xy}+\left.\frac{\partial f}{\partial \phi}\right|_{r\theta}\left.\frac{\partial \phi}{\partial z}\right|_{xy}\right)\hat{e}_z$$

We will need all the partial derivatives $\frac{\partial s_j}{\partial c_i}$. From $r^2 = x^2 + y^2 + z^2$ we see that

$$\left.\frac{\partial r}{\partial x}\right|_{yz} = \frac{x}{r} \qquad \left.\frac{\partial r}{\partial y}\right|_{xz} = \frac{y}{r} \qquad \left.\frac{\partial r}{\partial z}\right|_{xy} = \frac{z}{r}.$$

From $\cos\theta = z/r = z/\sqrt{x^2+y^2+z^2}$,

$$-\sin\theta\left.\frac{\partial \theta}{\partial x}\right|_{yz} = \frac{-zx}{\left(x^2+y^2+z^2\right)^{3/2}} = \frac{-r^2\cos\theta\sin\theta\cos\phi}{r^3}$$

so

$$\left.\frac{\partial \theta}{\partial x}\right|_{yz} = \frac{\cos\theta\cos\phi}{r}.$$

Similarly,

$$\left.\frac{\partial \theta}{\partial y}\right|_{xz} = \frac{\cos\theta\sin\phi}{r}.$$

There is an extra term when differentiating w.r.t. z, from the numerator, so

$$-\sin\theta\left.\frac{\partial \theta}{\partial z}\right|_{xy} = \frac{1}{r} - \frac{z^2}{r^3} = \frac{1-\cos^2\theta}{r} = r^{-1}\sin^2\theta,$$

so

$$\left.\frac{\partial \theta}{\partial z}\right|_{xy} = -r^{-1}\sin\theta.$$

Finally, the derivatives of ϕ can easily be found from differentiating $\tan\phi = y/x$. Using differentials,

$$\sec^2\phi d\phi = \frac{dy}{x} - \frac{ydx}{x^2} = \frac{dy}{r\sin\theta\cos\phi} - \frac{dx\sin\theta\sin\phi}{r\sin^2\theta\cos^2\phi}$$

so

$$\left.\frac{\partial\phi}{\partial x}\right|_{yz} = -\frac{1}{r}\frac{\sin\phi}{\sin\theta} \qquad \left.\frac{\partial\phi}{\partial y}\right|_{xz} = \frac{1}{r}\frac{\cos\phi}{\sin\theta} \qquad \left.\frac{\partial\phi}{\partial z}\right|_{xy} = 0.$$

Now we are ready to plug this all into (C.1). Grouping together the terms involving each of the three partial derivatives, we find

$$\begin{aligned}
\vec{\nabla} f &= \left.\frac{\partial f}{\partial r}\right|_{\theta\phi}\left(\frac{x}{r}\hat{e}_x + \frac{y}{r}\hat{e}_y + \frac{z}{r}\hat{e}_z\right) \\
&\quad + \left.\frac{\partial f}{\partial \theta}\right|_{r\phi}\left(\frac{\cos\theta\cos\phi}{r}\hat{e}_x + \frac{\cos\theta\sin\phi}{r}\hat{e}_y - \frac{\sin\theta}{r}\hat{e}_z\right) \\
&\quad + \left.\frac{\partial f}{\partial \phi}\right|_{r\theta}\left(-\frac{1}{r}\frac{\sin\phi}{\sin\theta}\hat{e}_x + \frac{1}{r}\frac{\cos\phi}{\sin\theta}\hat{e}_y\right) \\
&= \left.\frac{\partial f}{\partial r}\right|_{\theta\phi}\hat{e}_r + \frac{1}{r}\left.\frac{\partial f}{\partial \theta}\right|_{r\phi}\hat{e}_\theta + \frac{1}{r\sin\theta}\left.\frac{\partial f}{\partial \phi}\right|_{r\theta}\hat{e}_\phi
\end{aligned}$$

Thus we have derived the form for the gradient in spherical coordinates.

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Index