Chapter 3 Scalar Mechanics

In this chapter, we consider the reformulation of mechanics in which the **geometric** properties of vectors in three-dimensional space are not used. The emphasis shifts from components of vectors back to the coordinates of the particles within a system. We shall often bundle together several scalar quantities such as the coordinates of the particles into a single large vector, but this is purely for mathematical convenience and has no geometric significance. The space of permitted positions for all the particles in the system is known as **configuration space.**

3.1 Equilibrium of Systems

Before considering the problem of dynamics in which a system may be represented by a point which moves in configuration space, we wish to consider statics, in which the solution is a particular configuration of the system at which it is in equilibrium. The solution consists of one (or perhaps several) points in configuration space at which the total force on each particle vanishes.

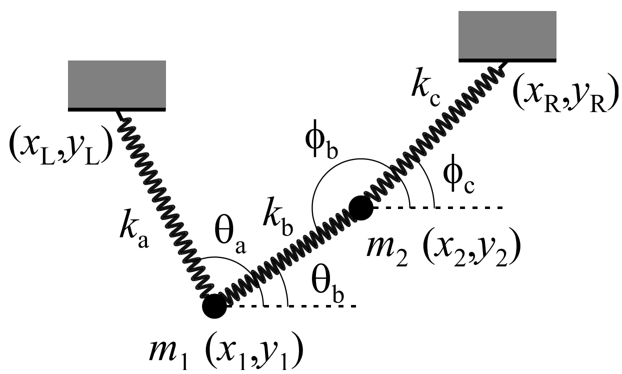

Figure 3.1 System of masses and springs in equilibrium

Consider the system shown in Figure 3.1 in which two masses are attached via three springs to the fixed positions (x_L, y_L) and (x_R, y_R) . Let the natural lengths of the springs be l_a, l_b and l_c and the spring constants be k_a, k_b and k_c. We wish to find the positions of the two masses such that the system is in equilibrium.

The vector approach to this problem involves finding the force on each mass due to gravity and the springs as a function of the positions (x_1, y_1) and (x_2, y_2) . The system is in equilibrium if the forces add up to zero. Since forces are vectors, this corresponds to making all the components add up to zero on each mass, leading to a system of simultaneous equations.

In the scalar approach, we calculate the potential energy of the system and find when this is a minimum. The potential energy can be split into two terms,

$$V(x_1, y_1, x_2, y_2) = V_{\text{ext}} + V_{\text{int}} \tag{3.1}$$

where V_{ext} is due to the external forces such as gravity and V_{int} is due to the internal forces of interaction. We wish to minimize V over positions in configuration space which we may denote by the four component "vector" $\mathbf{u}$, where

$$\mathbf{u} = \begin{pmatrix} x_1 \\ y_1 \\ x_2 \\ y_2 \end{pmatrix} \tag{3.2}$$

This should be regarded just as a collection of four numbers, written for convenience as a vector. The external potential energy is conveniently represented in terms of **u**, but the internal potential energy is more conveniently written in terms of the extensions of the springs, **e** where

$$\mathbf{e} = \begin{pmatrix} e_a \\ e_b \\ e_c \end{pmatrix} = \begin{pmatrix} \sqrt{(x_1 - x_L)^2 + (y_1 - y_L)^2} - l_a \\ \sqrt{(x_2 - x_1)^2 + (y_2 - y_1)^2} - l_b \\ \sqrt{(x_R - x_2)^2 + (y_R - y_2)^2} - l_c \end{pmatrix} \tag{3.3}$$

The relations $\mathbf{e}(\mathbf{u})$ are known as the "compatibility equations". The terms in the potential energy in this example are

$$V_{\text{ext}}(\mathbf{u}) = m_1 g y_1 + m_2 g y_2 \tag{3.4}$$

$$V_{\text{int}}(\mathbf{e}) = \frac{1}{2}k_a e_a^2 + \frac{1}{2}k_b e_b^2 + \frac{1}{2}k_c e_c^2 \tag{3.5}$$

Since we want to minimize V with respect to the positions $\mathbf{u}$, we need to use the compatibility equations to write

$$V(\mathbf{u}) = V_{\text{ext}}(\mathbf{u}) + V_{\text{int}}(\mathbf{e}(\mathbf{u})) \tag{3.6}$$

We use the chain rule to find the required derivatives

$$0 = -\frac{\partial V}{\partial u_j} = -\frac{\partial V_{\text{ext}}}{\partial u_j} + \sum_i \frac{\partial V_{\text{int}}}{\partial e_i}\left(-\frac{\partial e_i}{\partial u_j}\right) \tag{3.7}$$

Note that:

- The term $-\partial V_{\text{ext}}/\partial u_j$ is the component of the external force associated with the coordinate u_j. So for example, $-\partial V_{\text{ext}}/\partial y_1 = -m_1 g$ is the y component of the gravitational force on the first particle.
- The term $\partial V_{\text{int}}/\partial e_i$ is the tension in the spring i, so that for example, $\partial V_{\text{int}}/\partial e_a = k_a e_a$.
- The term $-\partial e_i/\partial u_j$ is a geometric factor which resolves the tension in spring i along the direction associated with the coordinate u_j. This partial derivative is non-zero only if spring i connects to the mass whose coordinate is u_j.

The following table shows the values of the various terms in the equation for $-\partial V/\partial u_j$

$-\frac{\partial V}{\partial u_j}$	=	$-\frac{\partial V_{\text{ext}}}{\partial u_j}$	+	$\frac{\partial V_{\text{int}}}{\partial e_a}\left(-\frac{\partial e_a}{\partial u_j}\right)$	+	$\frac{\partial V_{\text{int}}}{\partial e_b}\left(-\frac{\partial e_b}{\partial u_j}\right)$	+	$\frac{\partial V_{\text{int}}}{\partial e_c}\left(-\frac{\partial e_c}{\partial u_j}\right)$
$-\frac{\partial V}{\partial x_1}$	=	0	+	$k_a e_a \cos\theta_a$	+	$k_b e_b \cos\theta_b$	+	0
$-\frac{\partial V}{\partial y_1}$	=	$-m_1 g$	+	$k_a e_a \sin\theta_a$	+	$k_b e_b \sin\theta_b$	+	0
$-\frac{\partial V}{\partial x_2}$	=	0	+	0	+	$k_b e_b \cos\phi_b$	+	$k_c e_c \cos\phi_c$
$-\frac{\partial V}{\partial y_2}$	=	$-m_2 g$	+	0	+	$k_b e_b \sin\phi_b$	+	$k_c e_c \sin\phi_c$

Minimizing V by setting all of these derivatives eequal to zero is equivalent to summing the forces and making each component sum to zero.

3.2 Advantages of the Scalar Formulation

So far, we have seen that minimizing V over the configuration space is equivalent to solving the vector equations for force equilibrium. In this section we consider the advantages of expressing the solution of the equilibrium problem in terms of a minimization rather than in terms of the vector conditions for equilibrium.

Firstly, once we know that equilibrium holds when V is minimized, we can choose **any** coordinate system which determines the positions of the masses and express V in terms of these coordinates. For example, we may take r_1 to be the length of spring a, θ_1 to be the angle of spring a from the vertical, r_2 to be the length of spring b and θ_2 to be the angle of spring b from the vertical. Specifying the four numbers r_1, θ_1, r_2 and θ_2 also gives the positions of the two masses. Once we have expressed the potential energy in terms of these quantities $V(r_1, \theta_1, r_2, \theta_2)$, minimizing V with respect to these new variables by finding where

$$\frac{\partial V}{\partial r_1} = 0, \quad \frac{\partial V}{\partial \theta_1} = 0, \quad \frac{\partial V}{\partial r_2} = 0 \quad \text{and} \quad \frac{\partial V}{\partial \theta_2} = 0 \tag{3.8}$$

will also give the conditions for equilibrium, automatically expressed in terms of the new coordinates.

A second advantage is the way in which constraints can be included into the formulation. If the system is arranged so that not all positions of the masses are admissible, it is possible to find the (possibly new) new equilibrium configuration simply by minimizing V over the set of admissible configurations. For example, the system may be modified so that the mass m_2 is constrained to lie somewhere on a vertical line with a prescribed value of x_2. This could be arranged by cutting a vertical slot at this value of x_2 and forcing the mass m_2 to slide within this slot. Now instead of regarding V as a function of the four variables x_1, y_1, x_2 and y_2, the only free variables are x_1, y_1 and y_2, the value of x_2 having been fixed by the slot. We need to consider $V(x_1, y_1, y_2)$ and to minimize V with respect only to variations in these quantities. The minimizing conditions $\partial V/\partial x_1 = 0$, $\partial V/\partial y_1 = 0$ and $\partial V/\partial y_2 = 0$ correspond to the balance of forces in the horizontal and vertical directions at mass m_1, but only a vertical balance of forces at mass m_2. The horizontal components of the forces due to the springs acting on mass m_2 do not balance since the slot imposes an additional force of constraint in the x direction on this mass. Forces of constraint do not appear within the potential energy function and so we do not expect that $\partial V/\partial x_2 = 0$, unless by chance the slot happens to be in the position that m_2 would have occupied if it were unconstrained. In a vector formulation, it is usually the case that one has to compute all the forces of constraint before solving the problem, but this is usually not necessary in the scalar formulation.

It should also be apparent that when we are working with a constrained system, there may still be freedom in choosing a coordinate system that will map out the admissible configuration space. For example, in the example of the two masses and the vertical slot, it is possible to use r_1, θ_1 and y_2 rather than x_1, y_1 and y_2 as the three coordinates. In general, if $q_1, ..., q_s$ are any set of generalized coordinates which map out the admissible configuration space, solving the constrained problem requires us to find where $\partial V/\partial q_1 = 0, ..., \partial V/\partial q_s = 0$. The **number** of generalized coordinates needed to map out the admissible configuration space is a constant and is called the number of **degrees of freedom** of the system.

3.3 Dynamics in Coordinate Independent Form

In the case of statics, the condition of equilibrium may be expressed in terms of minimizing the potential energy V, and we found that the point at which this occurs may be found by using any generalized coordinate system $(q_1, ..., q_s)$ to describe the configuration space and finding where $\partial V/\partial q_i = 0$ for $i = 1, ..., s$. We shall see that in the case of dynamics, Newton's second law may be satisfied by using generalized coordinates $(q_1, ..., q_s)$ to describe the configuration space and solving the Lagrange equations

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}_j}\right) - \left(\frac{\partial L}{\partial q_j}\right) = 0 \tag{3.9}$$

for $j = 1, ..., s$ and where L is the Lagrangian of the system, given by the difference between the kinetic energy T and the potential energy V. In this section, we shall demonstrate that for unconstrained systems, Newton's laws lead to the Lagrange equations once a transformation into arbitrary generalized coordinates is made. The way in which constraints are included will be considered later.

From Newton's second law, the equations of motion in the inertial Cartesian frame are

$$\mathbf{F}_k = \frac{d}{dt}(m_k \dot{\mathbf{r}}_k) \tag{3.10}$$

which can be written in component form as the $3N$ equations

$$F_i = \frac{d}{dt}\left(m_i \dot{x}_i\right) \tag{3.11}$$

Note that for convenience, the masses have been relabelled in the second equation to accomodate the fact that three indicies are associated with each particle.

The kinetic energy of the system of particles is

$$T = \sum_{k=1}^{N} \frac{1}{2} m_k \dot{\mathbf{r}}_k^2 \tag{3.12}$$

which may also be rewritten as

$$T = \sum_{i=1}^{3N} \frac{1}{2} m_i \dot{x}_i^2 \tag{3.13}$$

The partial derivatives of T with respect to the velocity components are

$$\frac{\partial T}{\partial \dot{x}_i} = m_i \dot{x}_i \tag{3.14}$$

and so

$$\frac{d}{dt}\left(\frac{\partial T}{\partial \dot{x}_i}\right) = m_i \ddot{x}_i \tag{3.15}$$

If the system is **conservative**, the forces are derivable from a potential energy function V. In particular,

$$F_i = -\frac{\partial V}{\partial x_i} \tag{3.16}$$

Combining equations (3.15) and (3.16), we see that Newton's second law can be expressed in terms of the **scalar functions** T and V as

$$\frac{d}{dt}\left(\frac{\partial T}{\partial \dot{x}_i}\right) = -\frac{\partial V}{\partial x_i} \tag{3.17}$$

Note that we are assuming that T is a function of $\dot{x}_1, ..., \dot{x}_{3N}$ alone, while V is a function of $x_1, ..., x_{3N}$ alone.

Let us now consider what happens when we change from the inertial Cartesian coordinate system to the generalized coordinates. The kinetic and potential energies may be written in terms of the generalized coordinates as follows:

Since T depends on the velocities $\dot{x}_i$, and we know how x_i depends on the q_j, we can use the chain rule to calculate

$$\begin{aligned} \dot{x}_i &= \frac{d}{dt} x_i\left(q_1, ..., q_{3N}, t\right) \\ &= \frac{\partial x_i}{\partial q_1}\frac{dq_1}{dt} + ... + \frac{\partial x_i}{\partial q_{3N}}\frac{dq_{3N}}{dt} + \frac{\partial x_i}{\partial t} = \sum_{j=1}^{3N} \frac{\partial x_i}{\partial q_j}\dot{q}_j + \frac{\partial x_i}{\partial t} \end{aligned} \tag{3.18}$$

Notice that the partial derivatives $\partial x_i / \partial q_j$ will in general involve the q's and t. This means that the velocities $\dot{x}_i$ will be functions of both the q_j and the $\dot{q}_j$. as well as t. The kinetic energy may thus be written in terms of the generalized coordinates as $T\left(q_1, ..., q_{3N}, \dot{q}_1, ..., \dot{q}_{3N}, t\right)$. Notice that we are treating the quantities q_j and $\dot{q}_j$ as independent variables.

On the other hand, the potential energy (usually) depends only on the position coordinates $x_1, x_2, ..., x_{3N}$. When these are transformed, we find that V depends on $q_1, ..., q_{3N}$ and t. Thus we write $V\left(q_1, ..., q_{3N}, t\right)$.

We now look at the quantity

$$\frac{\partial T}{\partial \dot{q}_j} = \sum_{i=1}^{3N} \frac{\partial T}{\partial \dot{x}_i}\frac{\partial \dot{x}_i}{\partial \dot{q}_j} \tag{3.19}$$

From equation (3.18), we see that in this problem,

$$\frac{\partial \dot{x}_i}{\partial \dot{q}_j} = \frac{\partial x_i}{\partial q_j} \tag{3.20}$$

and so

$$\frac{\partial T}{\partial \dot{q}_j} = \sum_{i=1}^{3N} \frac{\partial T}{\partial \dot{x}_i} \frac{\partial x_i}{\partial q_j}. \tag{3.21}$$

If we consider the total derivative with respect to time,

$$\frac{d}{dt}\left(\frac{\partial T}{\partial \dot{q}_j}\right) = \sum_{i=1}^{3N} \frac{d}{dt}\left(\frac{\partial T}{\partial \dot{x}_i}\right)\frac{\partial x_i}{\partial q_j} + \frac{\partial T}{\partial \dot{x}_i}\frac{d}{dt}\left(\frac{\partial x_i}{\partial q_j}\right) \tag{3.22}$$

In the last term of this equation, x_i is a function of the q's and t alone. Thus, by the chain rule,

$$\begin{aligned} \frac{d}{dt}\left(\frac{\partial x_i}{\partial q_j}\right) &= \sum_{k=1}^{3N}\left(\frac{\partial^2 x_i}{\partial q_k\,\partial q_j}\right)\dot{q}_k + \frac{\partial^2 x_i}{\partial t\,\partial q_j} && (3.23)\\ &= \frac{\partial}{\partial q_j}\left\{\sum_{k=1}^{3N}\left(\frac{\partial x_i}{\partial q_k}\right)\dot{q}_k + \frac{\partial x_i}{\partial t}\right\} && (3.24)\\ &= \frac{\partial \dot{x}_i}{\partial q_j} && (3.25)\end{aligned}$$

where we have used (3.18) in the last equation. Substituting this and (3.17) into equation (3.22), we find

$$\begin{aligned} \frac{d}{dt}\left(\frac{\partial T}{\partial \dot{q}_j}\right) &= \sum_{i=1}^{3N}\left(-\frac{\partial V}{\partial x_i}\right)\frac{\partial x_i}{\partial q_j} + \frac{\partial T}{\partial \dot{x}_i}\frac{\partial \dot{x}_i}{\partial q_j} \\ &= -\frac{\partial V}{\partial q_j} + \frac{\partial T}{\partial q_j} && (3.26)\end{aligned}$$

This may be written as

$$\frac{d}{dt}\left(\frac{\partial T}{\partial \dot{q}_j}\right) - \frac{\partial T}{\partial q_j} = Q_j \tag{3.27}$$

where

$$Q_j = -\frac{\partial V}{\partial q_j} \tag{3.28}$$

is called the j'th **generalized force.**

3.3.1 Application to a Uniformly Rotating Coordinate System

As an illustrative example, let us consider the equations of motion of a single particle of mass m in the coordinate system q_1, q_2, q_3 which is related to the inertial Cartesian coordinate system $x_1 = x$, $x_2 = y$, $x_3 = z$ by the time-dependent transformation

$$\begin{aligned} q_1 &= x_1 \cos\omega t + x_2 \sin\omega t && (3.29)\\ q_2 &= -x_1 \sin\omega t + x_2 \cos\omega t && (3.30)\\ q_3 &= x_3 && (3.31)\end{aligned}$$

The inverse transformation is then

$$\begin{aligned} x_1 &= q_1 \cos\omega t - q_2 \sin\omega t && (3.32)\\ x_2 &= q_1 \sin\omega t + q_2 \cos\omega t && (3.33)\\ x_3 &= q_3 && (3.34)\end{aligned}$$

from which we can find

$$\begin{aligned}
\dot{x}_1 &= -(\dot{q}_2 + \omega q_1)\sin\omega t + (\dot{q}_1 - \omega q_2)\cos\omega t && (3.35)\\
\dot{x}_2 &= (\dot{q}_1 - \omega q_2)\sin\omega t + (\dot{q}_2 + \omega q_1)\cos\omega t && (3.36)\\
\dot{x}_3 &= \dot{q}_3 && (3.37)
\end{aligned}$$

We may write down the kinetic energy in terms of the new coordinates, which after simplification yields

$$T = \frac{1}{2}m\left((\dot{q}_2 + \omega q_1)^2 + (\dot{q}_1 - \omega q_2)^2 + \dot{q}_3^2\right) \qquad (3.38)$$

We then find

$$\begin{aligned}
\frac{d}{dt}\left(\frac{\partial T}{\partial \dot{q}_1}\right) - \frac{\partial T}{\partial q_1} &= m(\ddot{q}_1 - \omega\dot{q}_2) - m\omega(\dot{q}_2 + \omega q_1)\\
&= m\ddot{q}_1 - 2m\omega\dot{q}_2 - m\omega^2 q_1 && (3.39)\\
\frac{d}{dt}\left(\frac{\partial T}{\partial \dot{q}_2}\right) - \frac{\partial T}{\partial q_2} &= m(\ddot{q}_2 + \omega\dot{q}_1) + m\omega(\dot{q}_1 - \omega q_2)\\
&= m\ddot{q}_2 + 2m\omega\dot{q}_1 - m\omega^2 q_2 && (3.40)\\
\frac{d}{dt}\left(\frac{\partial T}{\partial \dot{q}_3}\right) - \frac{\partial T}{\partial q_3} &= m\ddot{q}_3 && (3.41)
\end{aligned}$$

so that in the generalized coordinate system, (3.27) becomes

$$\begin{aligned}
m\ddot{q}_1 - 2m\omega\dot{q}_2 - m\omega^2 q_1 &= Q_1 && (3.42)\\
m\ddot{q}_2 + 2m\omega\dot{q}_1 - m\omega^2 q_2 &= Q_2 && (3.43)\\
m\ddot{q}_3 &= Q_3 && (3.44)
\end{aligned}$$

We see that the rotating coordinate frame has introduced additional terms into Newton's second law from the derivatives $\partial T/\partial q_j$ (which are zero in the inertial frame). These may be identified as the Coriolis force and the centrifugal force discussed in the previous chapter, since q_1, q_2 and q_3 are just the components of the vector $\mathbf{r}_b$ considered there.

Exercise

Check that the above is consistent with

$$m\frac{d^2\mathbf{r}_b}{dt^2} + 2m\boldsymbol{\omega}\times\frac{d\mathbf{r}_b}{dt} + m\boldsymbol{\omega}\times(\boldsymbol{\omega}\times\mathbf{r}_b) = \mathbf{F}_b \qquad (3.45)$$

which was derived previously.

Exercise

Show that the equations of motion of a free particle (i.e., with no external applied forces) in spherical polar coordinates may be written as

$$\begin{aligned}
\ddot{r} &= r\left(\dot{\theta}^2 + \sin^2\theta\dot{\phi}^2\right) && (3.46)\\
\ddot{\theta} &= -\frac{2\dot{r}\dot{\theta}}{r} + (\sin\theta\cos\theta)\dot{\phi}^2 && (3.47)\\
\dot{\phi} &= \frac{\text{constant}}{r^2\sin^2\theta} && (3.48)
\end{aligned}$$

3.3.2 Lagrange's Equations

The set of equations (3.27) is a special case of **Lagrange's equations of motion**. Using the definition of the generalized force, we see that for a conservative system, they may be written equivalently as

$$\frac{d}{dt}\left(\frac{\partial T}{\partial \dot{q}_j}\right) - \frac{\partial T}{\partial q_j} = -\frac{\partial V}{\partial q_j} \qquad (3.49)$$

Since V is independent of the $\dot{q}_j$, if we define the **Lagrangian** to be

$$L = T - V \tag{3.50}$$

then the Lagrange equations of motion may be written as

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}_j}\right) - \frac{\partial L}{\partial q_j} = 0 \tag{3.51}$$

As we have seen above, a major advantage of using Lagrange's equations over Newton's equations is the ease with which arbitrary generalized coordinate systems may be treated. Although we have derived these equations so far for conservative systems without constraints, they are in fact true for more general systems. In particular, we shall show how certain types of constraints (so-called **holonomic** constraints) may be treated in a simple way, and that the effects of electromagnetic fields may also be placed within the Lagrangian framework if we allow V to depend on $\dot{q}_j$ as well as the q_j.

3.4 Constraints in Mechanics

For macroscopic systems, it is often the case that the motion is limited by one or more **constraints** which mean that not all functions $\mathbf{r}_k(t)$ which satisfy the endpoint conditions are permitted. Sometimes, it is possible to write these constraints in terms of **equations of constraint** which the coordinates have to satisfy during the motion. Such constraints are said to be **holonomic.** Examples of holonomic constraints are the constancy of the length of a pendulum or of the length of the string in a system of pullies. If we have a pendulum whose point of suspension is **a** and whose bob is at location $\mathbf{r}(t)$, the equation of constraint specifying that the length of the string is ℓ at all times is

$$(\mathbf{r}(t) - \mathbf{a}) \cdot (\mathbf{r}(t) - \mathbf{a}) = \ell^2 \tag{3.52}$$

Holonomic constraints are always specified by constraint equations which involve the coordinates (and possibly the time).

All other constraints are classified as non-holonomic. Examples of this include constraints that have to be represented as inequalities. Motion of a particle on a flat tabletop can usually be represented by the holonomic constraint $z = 0$, (where z is measured vertically upwards) but if there is the possibility that the particle will lift off the surface, this has to be replaced by the non-holonomic constraint $z \geq 0$. Another important class of non-holonomic constraint involves differential relations between the coordinates. For example, if a disc of radius a rolls without slipping on a horizontal plane, the distance ds that the point of contact moves when the disc turns through an angle $d\theta$ is given by $ds = a\,d\theta$. If the point of contact is (x, y), this may be written

$$\sqrt{dx^2 + dy^2} = a\,d\theta \tag{3.53}$$

but this cannot be integrated to give a holonomic constraint which relates the coordinates themselves.

When using the Lagrange equations of motion, it is easy to include the effects of holonomic constraints by reducing the number of generalized coordinates used to the number of degrees of freedom available to the system. For holonomic constraints, each (scalar) equation of constraint reduces the number of degrees of freedom by one, so that instead of using$3N$ (generalized) coordinates, it is possible to choose a reduced number of coordinates in such a way that the remaining $s = 3N - k$ functions (where k is the number of constraints) gives a solution which automatically satisfies the constraints. As a simple example, if we wish to describe the unconstrained motion of one particle in three-dimensional space, suitable coordinate systems would be (x, y, z), (r, θ, ϕ) or (ρ, ϕ, z). If we now consider the particle attatched to the origin via a string of length ℓ which remains taught during the motion, there are only two degrees of freedom, and the natural coordinate system for describing the motion would be the polar and azimuthal angles (θ, ϕ). Given θ and ϕ, the Cartesian coordinates of the particle would be $x = \ell \sin\theta \cos\phi$, $y = \ell \sin\theta \sin\phi$ and $z = \ell \cos\theta$. The advantage of using the coordinates (θ, ϕ) is that **any** motion satisfying the constraint can be represented by the functions $\theta(t)$ and $\phi(t)$ and conversely, given any functions $\theta(t)$ and $\phi(t)$, the trajectory defined by those functions will satisfy the constraint. If we express the Lagrangian and the action in terms of $\theta(t)$ and $\phi(t)$, the Lagrange equations automatically give us the equations of motion of the constrained system.

When the constraints are non-holonomic, it is not possible to tailor a system of generalized coordinates which map out the configuration space. In this case, it is sometimes possible to use Lagrange multiplier techniques, but we shall delay discussion of this topic until later. For the moment, we shall proceed to applying Lagrange's equations to systems with holonomic constraints in order to become more familiar with the techniques involved.

3.5 Examples of Use of Lagrange's Equations

3.5.1 Motion in a vertical plane under gravity

Consider a particle of mass m in a gravitational field with Cartesian coordinates (x, y) where y is directed vertically upwards. The Lagrangian is given by

$$L = T - V = \frac{1}{2}m\left(\dot{x}^2 + \dot{y}^2\right) - mgy \tag{3.54}$$

Lagrange's equations are

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}_j}\right) - \left(\frac{\partial L}{\partial q_j}\right) = 0 \tag{3.55}$$

We see that in this case, L is independent of the coordinate x and so $\partial L/\partial x = 0$. As a consequence,

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{x}}\right) = 0 \tag{3.56}$$

and so $\partial L/\partial \dot{x}$ is independent of time. The coordinates x is then said to be **ignorable** or **cyclic.** Using the expression for the Lagrangian, this means that

$$\frac{\partial L}{\partial \dot{x}} = m\dot{x} \tag{3.57}$$

is a constant of the motion. For the y coordinate, we find that

$$\frac{d}{dt}(m\dot{y}) + mg = 0 \tag{3.58}$$

or

$$\ddot{y} = -g \tag{3.59}$$

Using the initial conditions, we obtain the familiar solutions

$$x(t) = x(0) + \dot{x}(0)\,t \tag{3.60}$$

$$y(t) = y(0) + \dot{y}(0)\,t - \frac{1}{2}gt^2 \tag{3.61}$$

3.5.2 Motion of a Pendulum in a Vertical plane

This uses the same Lagrangian as for the above problem, but we impose the constraint that the length of the pendulum remains constant by using a single angular coordinate to specify the position of the bob. If the length of the string is ℓ and the point of suspension is the origin, we can define θ to be the angle to the vertical so that

$$x = \ell\sin\theta \tag{3.62}$$

$$y = -\ell\cos\theta \tag{3.63}$$

The Lagrangian (3.54) can be rewritten in terms of the coordinate θ and its derivative as

$$L = \frac{1}{2} m \ell^2 \dot{\theta}^2 + mg\ell \cos\theta \tag{3.64}$$

Calculating derivatives, we find

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{\theta}}\right) = m\ell^2 \ddot{\theta} \tag{3.65}$$

$$\frac{\partial L}{\partial \theta} = -mg\ell \sin\theta \tag{3.66}$$

and so

$$\ddot{\theta} = -\frac{g}{\ell} \sin\theta \tag{3.67}$$

which is the usual equation of motion for a pendulum. Notice that we have not needed to compute the tension in the string in this calculation. The difference between this solution and the previous one originates entirely from using a coordinate system which respects the constrained configuration space of the system.

3.5.3 Atwood's Machine

This is the name given to the problem of two masses m_1 and m_2 connected via a string of constant length passing over a frictionless pulley. If x_1 is the height of mass m_1 and x_2 is the height of mass m_2, we note that when one mass goes up, the other mass goes down by the same amount. Thus the constraint that the string is of constant length may be written as $x_1 + x_2 = c$ for some constant c. It is clear that the constraint makes the system have only one degree of freedom, and so we can introduce the single generalized coordinate q from which both x_1 and x_2 may be calculated via

$$x_1 = q \quad \text{and} \quad x_2 = c - q \tag{3.68}$$

The Lagrangian is given by

$$L = \frac{1}{2} m_1 \dot{x}_1^2 + \frac{1}{2} m_2 \dot{x}_2^2 - m_1 g x_1 - m_2 g x_2 \tag{3.69}$$

which may be written in terms of q and $\dot{q}$ as

$$L = \frac{1}{2} m_1 \dot{q}^2 + \frac{1}{2} m_2 \dot{q}^2 - m_1 g q - m_2 g (c - q) \tag{3.70}$$

Calculating derivatives, we find

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}}\right) = (m_1 + m_2)\, \ddot{q} \tag{3.71}$$

$$\left(\frac{\partial L}{\partial q}\right) = (m_2 - m_1)\, g \tag{3.72}$$

so that Lagrange's equation is

$$(m_1 + m_2)\, \ddot{q} = (m_2 - m_1)\, g \tag{3.73}$$

or

$$\ddot{q} = \frac{m_2 - m_1}{m_1 + m_2} g \tag{3.74}$$

which is exactly what we would expect from elementary considerations.

3.5.4 Door with a Non-vertical Hinge

Consider a thin door of height ℓ and width a of uniform mass per unit area ρ which is mounted on a hinge whose axis lies in the yz pland makes an angle θ with the vertical z. Let ϕ denote the angle between the door and the yz plane. We wish to consider the motion of the door and to show that it can undergo small oscillations.

The only degree of freedom in this problem is the angle ϕ, which we shall use as the generalized coordinate. The kinetic energy of the door is found by integrating over the mass distribution of the door. Consider the portion of the door between r and $r + \delta r$ away from the hinge. Its velocity is given by $r\dot{\phi}$ and its mass is $\rho\ell\, dr$. Thus the total kinetic energy is

$$T = \frac{1}{2}\int_0^a dr\, \rho\ell \left(r\dot{\phi}\right)^2 = \frac{a^3}{6}\rho\ell\dot{\phi}^2 \tag{3.75}$$

The potential energy of the door is most easily found by locating the position of its centre of mass, which by symmetry is in the centre of the door. If we consider the zero of potential energy to be at the height of the centre of the door when it is closed, i.e., when $\phi = 0$ we see that the effect of opening the door by angle ϕ is to raise its centre of mass by a height $\frac{1}{2}a(1 - \cos\phi)\sin\theta$. Since the mass of the door is $\rho\ell a$, we see that

$$V = \frac{1}{2}\rho\ell a^2 g (1 - \cos\phi)\sin\theta \tag{3.76}$$

The Lagrangian is given by

$$L = T - V = \frac{a^3}{6}\rho\ell\dot{\phi}^2 - \frac{1}{2}\rho\ell a^2 g(1 - \cos\phi)\sin\theta \tag{3.77}$$

from which we calculate

$$\frac{d}{dt}\left(\frac{\partial L}{\partial\dot{\phi}}\right) = \frac{a^3}{3}\rho\ell\ddot{\phi} \tag{3.78}$$

$$\frac{\partial L}{\partial\phi} = -\frac{1}{2}\rho\ell a^2 g\sin\phi\,\sin\theta \tag{3.79}$$

so that Lagrange's equation becomes

$$\frac{a^3}{3}\rho\ell\ddot{\phi} = -\frac{1}{2}\rho\ell a^2 g\sin\phi\,\sin\theta \tag{3.80}$$

or

$$\ddot{\phi} = -\frac{3g\sin\theta}{2a}\sin\phi \tag{3.81}$$

If ϕ is small so that we may approximate $\sin\phi \approx \phi$, this corresponds to simple harmonic motion about the equilibrium position $\phi = 0$ with angular frequency

$$\omega = \sqrt{\frac{3g\sin\theta}{2a}}. \tag{3.82}$$

3.5.5 Motion of a Bead on a Rotating Wire

Consider a cylindrical polar coordinate system (ρ, ϕ, z) and a wire which is bent into a curve $z = f(\rho)$ which lies within a plane. The wire rotates about the z axis with constant angular velocity ω. The problem is to find the equation of the curve such that a bead of mass m placed at any point on the wire remains stationary as the wire is rotated.

Again, this is a problem with only one degree of freedom, namely the position of the bead on the (one-dimensional) wire. For convenience, we can choose this to be the ρ coordinate. The other two coordinates are specified by the constraints and are thus given by

$$\phi = \omega t \tag{3.83}$$

$$z = f(\rho) \tag{3.84}$$

In this case, the transformation equations between the generalized coordinate and the inertial coordinates are time-dependent. The kinetic energy is given by

$$T = \frac{1}{2}m\left(\dot{\rho}^2 + \rho^2\dot{\phi}^2 + \dot{z}^2\right) \tag{3.85}$$

$$= \frac{1}{2}m\left(\dot{\rho}^2 + \rho^2\omega^2 + \{f'(\rho)\,\dot{\rho}\}^2\right) \tag{3.86}$$

and the potential energy is

$$V = mgz = mgf(\rho) \tag{3.87}$$

so that the Lagrangian is

$$L = T - V = \frac{1}{2}m\left(\dot{\rho}^2 + \rho^2\omega^2 + \{f'(\rho)\dot{\rho}\}^2\right) - mgf(\rho) \tag{3.88}$$

Calculating the derivatives, we find

$$\frac{\partial L}{\partial \dot{\rho}} = m\left\{1 + f'(\rho)^2\right\}\dot{\rho} \tag{3.89}$$

and

$$\frac{\partial L}{\partial \rho} = m\rho\omega^2 + mf'(\rho)f''(\rho)\dot{\rho}^2 - mgf'(\rho) \tag{3.90}$$

Lagrange's equations of motion thus have the form

$$\frac{d}{dt}\left(\left\{1 + f'(\rho)^2\right\}\dot{\rho}\right) = \rho\omega^2 + f'(\rho)f''(\rho)\dot{\rho}^2 - gf'(\rho) \tag{3.91}$$

Evaluating the derivative on the left hand side yields

$$\frac{d}{dt}\left(\left\{1 + f'(\rho)^2\right\}\dot{\rho}\right) = \left\{1 + f'(\rho)^2\right\}\ddot{\rho} + 2f'(\rho)f''(\rho)\dot{\rho}^2 \tag{3.92}$$

and so the equations of motion reduce to

$$\left\{1 + f'(\rho)^2\right\}\ddot{\rho} + f'(\rho)f''(\rho)\dot{\rho}^2 - \rho\omega^2 + gf'(\rho) = 0 \tag{3.93}$$

If we require that the bead remain stationary on the wire, ρ is constant and hence $\dot{\rho} = 0$ and $\ddot{\rho} = 0$. This leads to

$$-\rho\omega^2 + gf'(\rho) = 0 \tag{3.94}$$

or

$$\frac{df}{d\rho} = \frac{\omega^2}{g}\rho \tag{3.95}$$

which may be integrated to give

$$f(\rho) = \frac{\omega^2\rho^2}{2g} + \text{constant} \tag{3.96}$$

and so the wire needs to be bent into the shape of a parabola. The equation of motion then reduces to

$$\left\{1 + f'(\rho)^2\right\}\ddot{\rho} + f'(\rho)f''(\rho)\dot{\rho}^2 = 0 \tag{3.97}$$

for which $\rho =$constant is a solution.

The fact that a bead will remain stationary on a rotating wire bent in this way indicates that the force **along** the wire vanishes. We can see this more clearly by changing the coordinate to s, the distance of the bead from the centre of rotation measured along the wire. Since the wire remains in the $z\rho$ plane, we may write

$$ds^2 = d\rho^2 + dz^2 \tag{3.98}$$

Since the shape of the wire is given by $z = f(\rho)$, the increments $d\rho$ and dz are not independent for the bead moving on the wire. Indeed, $dz = f'(\rho)\, d\rho$ and so

$$ds = \sqrt{1 + f'(\rho)^2}\, d\rho \tag{3.99}$$

Thus

$$\dot{s} = \sqrt{1 + f'(\rho)^2}\,\dot{\rho} \tag{3.100}$$

$$\ddot{s} = \frac{f'(\rho)f''(\rho)}{\sqrt{1 + f'(\rho)^2}}\dot{\rho}^2 + \sqrt{1 + f'(\rho)^2}\,\ddot{\rho} \tag{3.101}$$

and so

$$\sqrt{1+f'(\rho)^2}\;\ddot{s} = \left\{1+f'(\rho)^2\right\}\ddot{\rho} + f'(\rho)\,f''(\rho)\,\dot{\rho}^2 \tag{3.102}$$

Comparing this with equation (3.97), we see that when $f(\rho)$ is given by (3.97) the equation of motion in terms of s is simply

$$\ddot{s} = 0 \tag{3.103}$$

which has solution

$$s = s_0 + v_0 t \tag{3.104}$$

corresponding to the bead being at rest or to uniform motion along the length of the wire.

3.6 Lagrange Equations and Conservation Laws

From the Lagrange equations

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}_j}\right) - \frac{\partial L}{\partial q_j} = 0 \tag{3.105}$$

we see that if L happens to be independent of q_j so that q_j is cyclic or ignorable, then if we define

$$p_j \equiv \frac{\partial L}{\partial \dot{q}_j} \tag{3.106}$$

it follows that p_j is a constant of the motion. The quantity p_j is known as the momentum conjugate to q_j. This allows us to identify quantities which are conserved during the dynamics. If H is independent of q_j, then its conjugate momentum p_j is conserved.

As an example consider a body of mass m_2 moving on the surface of a smooth table and connected via a light string of length l which passes without friction through a hole located at the centre of the table. Attached to the string is a mass m_1 which hangs vertically under the table. If r is the length of the string from the centre of the table to m_2, and θ is the angle that the string on the surface of the table makes to some reference, the Lagrangian is given by

$$L = \frac{1}{2}m_1\dot{r}^2 + \frac{1}{2}m_2\left(\dot{r}^2 + r^2\dot{\theta}^2\right) + m_1 g\,(l-r) \tag{3.107}$$

Since this is independent of θ, θ is an ignorable coordinate and its conjugate momentum p_θ is conserved:

$$p_\theta = \frac{\partial L}{\partial \dot{\theta}} = m_2 r^2\dot{\theta} \tag{3.108}$$

This may be identified as the angular momentum of m_2 taken about the hole in the table. Thus the invariance of L with respect to rotation leads to the existence of a conserved angular momentum.

An interesting situation occurs if L is not an explicit function of the time t, i.e., if $\partial L/\partial t = 0$. The time-derivative of L following the motion of the system is given by

$$\frac{dL}{dt} = \sum_{j=1}^{s}\left(\frac{\partial L}{\partial q_j}\dot{q}_j + \frac{\partial L}{\partial \dot{q}_j}\ddot{q}_j\right) + \frac{\partial L}{\partial t} \tag{3.109}$$

Using the Lagrange equations, this may be written as

$$\begin{aligned}\frac{dL}{dt} &= \sum_{j=1}^{s}\left\{\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}_j}\right)\dot{q}_j + \frac{\partial L}{\partial \dot{q}_j}\ddot{q}_j\right\} + \frac{\partial L}{\partial t} &(3.110)\\ &= \frac{d}{dt}\left(\sum_{j=1}^{M}\frac{\partial L}{\partial \dot{q}_j}\dot{q}_j\right) + \frac{\partial L}{\partial t} &(3.111)\end{aligned}$$

Now if V is independent of $\dot{q}_j$ and if T is a homogeneous quadratic form of $\dot{q}_j$, i.e., if

$$T = \sum_{k=1}^{s} \sum_{l=1}^{s} a_{kl}\,(q_1, ..., q_s)\,\dot{q}_k \dot{q}_l \tag{3.112}$$

then

$$\frac{d}{dt}\left(\sum_{j=1}^{s} \frac{\partial L}{\partial \dot{q}_j}\dot{q}_j\right) = \frac{d}{dt}\left(\sum_{j=1}^{s} \frac{\partial T}{\partial \dot{q}_j}\dot{q}_j\right) = 2\frac{dT}{dt} \tag{3.113}$$

and so

$$\frac{dL}{dt} = \frac{d\,(T-V)}{dt} = 2\frac{dT}{dt} + \frac{\partial L}{\partial t} \tag{3.114}$$

whence

$$\frac{d}{dt}\,(T+V) = -\frac{\partial L}{\partial t}. \tag{3.115}$$

So if L is not explicitly dependent on t, $\partial L/\partial t = 0$ and the total energy $T + V$ is conserved.

3.7 Velocity-dependent Potentials

In our original derivation of Lagrange equations of motion (3.27),

$$\frac{d}{dt}\left(\frac{\partial T}{\partial \dot{q}_j}\right) - \frac{\partial T}{\partial q_j} = Q_j = -\frac{\partial V}{\partial q_j}, \tag{3.116}$$

after introducing the Lagrangian $L = T - V$, we rewrote the equation in terms of L, leading to (3.51) which is equivalent to

$$\frac{d}{dt}\left(\frac{\partial T}{\partial \dot{q}_j}\right) - \frac{\partial T}{\partial q_j} = \frac{d}{dt}\left(\frac{\partial V}{\partial \dot{q}_j}\right) - \frac{\partial V}{\partial q_j} \tag{3.117}$$

so that in effect, the definition of the generalized force has been changed to

$$Q_j = \frac{d}{dt}\left(\frac{\partial V}{\partial \dot{q}_j}\right) - \frac{\partial V}{\partial q_j} \tag{3.118}$$

For all the conservative systems which we have considered so far, V has been independent of the generalized velocities $\dot{q}_j$ and so this reduces to the equations given previously. However, it turns out that it is sometimes useful to allow V to be velocity-dependent and to see what the resulting forces turn out to be. It is found that by making suitable a choice for V, it is possible to include electrodynamics into the Lagrangian framework as follows:

Suppose that there is a charged particle moving in a region in which there is an electric field $\mathbf{E}$ and a magnetic field $\mathbf{B}$. The force on the charge e due to the electromagnetic field is given by the Lorentz force

$$\mathbf{F} = e\,(\mathbf{E} + \mathbf{v} \times \mathbf{B}) \tag{3.119}$$

The fields are related to the scalar and vector potentials ϕ and $\mathbf{A}$ via the usual relationships

$$\mathbf{E} = -\boldsymbol{\nabla}\phi - \frac{\partial \mathbf{A}}{\partial t} \tag{3.120}$$

$$\mathbf{B} = \boldsymbol{\nabla} \times \mathbf{A} \tag{3.121}$$

We shall show that if we define the velocity-dependent potential

$$V = e\phi - e\mathbf{v}\cdot\mathbf{A} \tag{3.122}$$

then the derivative in Lagrange's equation

$$Q_j = \frac{d}{dt}\left(\frac{\partial V}{\partial \dot{q}_j}\right) - \frac{\partial V}{\partial q_j} \tag{3.123}$$

correctly recovers the generalized force. It suffices to show this for Cartesian coordinates and to appeal to Hamilton's principle for other choices of generalized coordinates.

Let us consider the x component. We then need to consider $\partial V/\partial \dot{x}$ and $\partial V/\partial x$. Since $V = e\phi - e\dot{x}A_x - e\dot{y}A_y - e\dot{z}A_z$, we see that

$$\frac{d}{dt}\left(\frac{\partial V}{\partial \dot{x}}\right) = -e\frac{dA_x}{dt} \tag{3.124}$$

and

$$\frac{\partial V}{\partial x} = e\frac{\partial \phi}{\partial x} - e\frac{dx}{dt}\frac{\partial A_x}{\partial x} - e\frac{dy}{dt}\frac{\partial A_y}{\partial x} - e\frac{dz}{dt}\frac{\partial A_z}{\partial x} \tag{3.125}$$

In equation (3.124), the time derivative of A_x is computed following the motion of the charged particle. Since the particle is moving in the field,

$$\frac{dA_x}{dt} = \frac{dx}{dt}\frac{\partial A_x}{\partial x} + \frac{dy}{dt}\frac{\partial A_x}{\partial y} + \frac{dz}{dt}\frac{\partial A_x}{\partial z} + \frac{\partial A_x}{\partial t} \tag{3.126}$$

Substituting these into Lagrange's equation,

$$\begin{aligned}
\frac{d}{dt}\left(\frac{\partial V}{\partial \dot{x}}\right) - \frac{\partial V}{\partial x} &= -e\left\{\frac{dy}{dt}\frac{\partial A_x}{\partial y} + \frac{dz}{dt}\frac{\partial A_x}{\partial z} + \frac{\partial A_x}{\partial t}\right\} - e\frac{\partial \phi}{\partial x} + e\frac{dy}{dt}\frac{\partial A_y}{\partial x} + e\frac{dz}{dt}\frac{\partial A_z}{\partial x} &(3.127)\\
&= e\frac{dy}{dt}\left(\frac{\partial A_y}{\partial x} - \frac{\partial A_x}{\partial y}\right) - e\frac{dz}{dt}\left(\frac{\partial A_x}{\partial z} - \frac{\partial A_z}{\partial x}\right) - e\frac{\partial \phi}{\partial x} - e\frac{\partial A_x}{\partial t} &(3.128)
\end{aligned}$$

Recalling that

$$\begin{aligned}
\mathbf{B} &= \nabla \times \mathbf{A} = \left(\frac{\partial A_z}{\partial y} - \frac{\partial A_y}{\partial z}, \frac{\partial A_x}{\partial z} - \frac{\partial A_z}{\partial x}, \frac{\partial A_y}{\partial x} - \frac{\partial A_x}{\partial y}\right) &(3.129)\\
\mathbf{E} &= -\nabla \phi - \frac{\partial \mathbf{A}}{\partial t} = \left(-\frac{\partial \phi}{\partial x} - \frac{\partial A_x}{\partial t}, -\frac{\partial \phi}{\partial y} - \frac{\partial A_y}{\partial t}, -\frac{\partial \phi}{\partial z} - \frac{\partial A_z}{\partial t}\right) &(3.130)
\end{aligned}$$

$$\frac{d}{dt}\left(\frac{\partial V}{\partial \dot{x}}\right) - \frac{\partial V}{\partial x} = e\left(v_y B_z - v_z B_y\right) + eE_x = e\left(\mathbf{E} + \mathbf{v} \times \mathbf{B}\right)_x \tag{3.131}$$

and so we have recovered the Lorentz force equation from the Lagrange equation.

3.7.1 Larmor's Theorem

Let us consider the problem of single-particle electrodynamics in the presence of a constant $\mathbf{B}$ field, which we may assume to be oriented in the z direction, i.e., $\mathbf{B} = B\hat{\mathbf{z}}$. As a typical example, consider a single electron of charge $q = -e$ attracted to a nucleus of charge $Q = Ze$ which is sufficiently massive that it may be regarded as being at rest. The nucleus is assumed to provide a static Coulomb potential in which the electron moves. The Lagrangian is

$$L = T - V = T + \frac{Ze^2}{4\pi\varepsilon_0 r} - e\mathbf{v}\cdot\mathbf{A} \tag{3.132}$$

where r is the distance of the electron from the nucleus, $\mathbf{v}$ is the velocity of the electron and $\mathbf{A}$ is the magnetic vector potential. If we work in cylindrical polar coordinates, we can set

$$\mathbf{A} = \frac{1}{2}B\rho\hat{\boldsymbol{\phi}} \tag{3.133}$$

to represent the uniform $\mathbf{B}$ field in the z direction (since $\nabla \times \mathbf{A} = (0, 0, B)$).

Since $\mathbf{v} = \dot{\rho}\hat{\boldsymbol{\rho}} + \rho\dot{\phi}\hat{\boldsymbol{\phi}} + \dot{z}\hat{\mathbf{z}}$, the Lagrangian may be written as

$$L = \frac{1}{2}m\left(\dot{\rho}^2 + \rho^2\dot{\phi}^2 + \dot{z}^2\right) + \frac{Ze^2}{4\pi\varepsilon_0\sqrt{\rho^2 + z^2}} - e\left(\frac{1}{2}B\rho\right)\left(\rho\dot{\phi}\right). \tag{3.134}$$

We observe that L is independent of ϕ, so that p_ϕ is conserved. In this situation,

$$p_\phi = \frac{\partial L}{\partial \dot{\phi}} = m\rho^2\dot{\phi} - \frac{eB}{2}\rho^2 = m\rho^2\left(\dot{\phi} - \frac{eB}{2m}\right) \tag{3.135}$$

The quantity $eB/(2m)$ is known as the Larmor frequency and is denoted by ω_L. Since p_ϕ is constant, this means that

$$m\rho^2\left(\dot{\phi} - \omega_L\right) \tag{3.136}$$

is constant. This may be contrasted with the situation for the central force problem in the absence of a magnetic field where $m\rho^2\dot{\phi}$ is constant.

Now consider using a new set of coordinates ρ, ϕ', z where $\phi' = \phi - \omega_L t$. In terms of these coordinates,

$$L = \frac{1}{2}m\left[\dot{\rho}^2 + \rho^2\left(\dot{\phi}' + \omega_L\right)^2 + \dot{z}^2\right] + \frac{Ze^2}{4\pi\varepsilon_0\sqrt{\rho^2+z^2}} - m\omega_L\rho^2\left(\dot{\phi}' + \omega_L\right) \tag{3.137}$$

$$= \frac{1}{2}m\left[\dot{\rho}^2 + \rho^2\left(\dot{\phi}'^2 + \omega_L^2\right) + \dot{z}^2\right] + \frac{Ze^2}{4\pi\varepsilon_0\sqrt{\rho^2+z^2}} \tag{3.138}$$

For a magnetic field of $\approx 1\,\mathrm{T}$ and a typical atomic orbit, we find that $\omega_L/\dot{\phi}' \approx 10^{-6}$ and so we can neglect ω_L^2 in comparison with $\dot{\phi}'^2$. The Lagrangian is then identical to that with no magnetic field, and so we can use the solutions for motion without a magnetic field and to realize that these apply in a frame which is rotating at ω_L.

3.8 The Action Principle (Hamilton's Principle)

The action principle is a formulation of mechanics in terms of a variational principle, analogous to the statement that a mechanical system is in equilibrium if the configuration minimizes the potential energy. We shall describe the action principle and show how solving it leads to the Lagrange equations of motion. An advantage of deriving the Lagrange equations of motion in this way is the simplicity with which constraints may be included in the formalism.

For a system of particles whose configuration space is parameterized in terms of the s generalized coordinates $q_1, ..., q_s$ a **trajectory** (or **path)** in configuration space on the interval of time $[t_1, t_2]$ is a collection of functions $q_1(t), ..., q_s(t)$ which specify how the configuration of the system evolves over this interval. The **action** associated with this trajectory is defined to be

$$S(q_1, q_2, ..., q_s) = \int_{t_1}^{t_2} L(q_1, ..., q_s, \dot{q}_1, ..., \dot{q}_s, t)\, dt \tag{3.139}$$

Once the functions $q_1, ..., q_s$ are specified, the action is just a number. Thus S is a "machine" which takes as its input the s functions $q_1(t), ..., q_s(t)$ and returns a number, $S(q_1, q_2, ..., q_s)$. Such a machine is known as a **functional.**

The **action principle** (sometimes called Hamilton's principle or the principle of least action) asserts that out of all the permitted trajectories that the particles of the system can take between a specified initial configuration at time t_1 and a specified final configuration at time t_2, they take the path(s) for which the action S has an extreme value (usually a minimum).

Features of the action principle are that:

1. All other equations of motion such as Newton's laws and the Lagrange equations of motion may be derived from the action principle,

2. The formulation is (almost) self-evidently coordinate independent, since a change in coordinates only changes our **description** of the set of possible trajectories over which the computation of the extremum has to be performed. The trajectory (or trajectories) at which the extreme value is attained is independent of the way we choose to describe it, and so the resulting solution found in any coordinate system describes the same physical dynamical evolution.

3. It is straightforward to include constraints by restricting the space of functions over which the extremum is computed to those which satisfy the constraints. In principle, both holonomic and non-holonomic constraints may be treated in this way, although in practice the restriction of the function space can be difficult to express in a way which allows a solution to be computed.

The action principle is an example of a **variational principle** which is one which involves finding the extreme value of a quantity over a set of some sort. In the past, we have mainly considered sets of points in spaces of finite dimension, but the action principle requires the extreme value to be computed over a set of functions. We shall consider via a set of examples how the techniques of calculus may be extended to those of the calculus of variations, which are required to treat the extremization of functionals.

3.8.1 Minimization of a function of several variables

Let us consider first the minimization of a function such as the potential energy $V(q_1,...,q_s)$ where $q_1,...,q_s$ are here regarded as specifying a **point** in s dimensions. The **variation** in the function δV when the point is varied from $q=(q_1,...,q_s)$ to $q+\delta q=(q_1+\delta q_1,...,q_s+\delta q_s)$ is defined to be

$$\delta V = V(q_1+\delta q_1,...,q_s+\delta q_s) - V(q_1,...,q_s) \tag{3.140}$$

Provided that V is sufficiently differentiable, we may express δV in terms of the variations of the variables δq_j via Taylor's theorem:

$$\delta V \approx \left(\frac{\partial V}{\partial q_1}\,\delta q_1 + ... + \frac{\partial V}{\partial q_s}\,\delta q_s\right) + \frac{1}{2!}\sum_{k=1}^{s}\sum_{l=1}^{s}\frac{\partial^2 V}{\partial q_k \partial q_l}\,\delta q_k\,\delta q_l + ... \tag{3.141}$$

The term in parentheses is known as the first-order variation since it is linear in δq, the second term is the second-order variation since it is quadratic in δq and so on. The condition for the point q to be an extremum is that the first-order variation vanishes. This means that for any variation δq about q the change in δV must be of at least second-order in δq. Since each of the components q_j of q may be varied independently, we require all the first order partial derivatives vanish, i.e., $\partial v/\partial q_j = 0$ for $j = 1,...,s$. It is this idea of the vanishing of the first-order variation which allows us to treat the more complicated situation of the minimization of functionals.

3.8.2 Minimization of a functional involving a single function

Let us now consider the minimization of a functional $I(x)$ which returns for a function $x:[a,b]\to\mathbb{R}$, a number computed according to the rule

$$I(x) = \int_a^b F(t,x,\dot{x})\,dt \text{ where } \dot{x} \equiv \frac{dx}{dt} \tag{3.142}$$

where $F:\mathbb{R}^3\to\mathbb{R}$ is a specified function. The function $x(t)$ is an extremum of the functional I means that if x is varied by δx, where $\delta x:[a,b]\to\mathbb{R}$ is also a function defined on the same interval, the variation δI in I, where

$$\delta I = I(x+\delta x) - I(x) \tag{3.143}$$

vanishes to first order in δx. As we shall see, it is important when framing such a problem to specify exactly what sorts of variation δx are to be allowed.

Consider the following specific example of minimizing of a functional. The arc length along the graph $x(t)$ from a to b is given by the integral

$$\text{Arc length} = \int_a^b \sqrt{1 + \left(\frac{dx}{dt}\right)^2}\, dt \tag{3.144}$$

In this case, the function $F(t, x, \dot{x})$ is

$$F(t, x, \dot{x}) = \sqrt{1 + \dot{x}^2} \tag{3.145}$$

Let us use variational calculus to find the curve of minimum length which passes through the points (a, c) and (b, d). It is obvious in this case that the solution is a straight line joining these points, but it is interesting to see how this arises from the formalism.

If we want the curve to pass through the specified points, we require that $x(a) = c$ and $x(b) = d$. The curve after applying a variation is specified by the function $x(t) + \delta x(t)$. Unless we state that $\delta x(a) = 0$ and $\delta x(b) = 0$, we cannot be sure that the "candidate" function $x + \delta x$ will still pass through the desired endpoints. Other than this, however, the vaules of δx at points t within the open interval (a, b) are arbitrary.

The variation in the functional $I(x)$ is

$$\begin{aligned} \delta I(x) &= I(x + \delta x) - I(x) = \int_a^b [F(t, x + \delta x, \dot{x} + \delta \dot{x}) - F(t, x, \dot{x})]\, dt & (3.146) \\ &= \int_a^b \left(\frac{\partial F}{\partial x}\delta x + \frac{\partial F}{\partial \dot{x}}\delta \dot{x}\right) dt + \text{ terms of higher order in } \delta x & (3.147) \end{aligned}$$

We may use integration by parts to convert the term involving $\delta \dot{x}$ to one involving δx

$$\delta I = \left[\delta x(t)\frac{\partial F}{\partial \dot{x}}(t)\right]_a^b + \int_a^b \left\{\frac{\partial F}{\partial x} - \frac{d}{dt}\left(\frac{\partial F}{\partial \dot{x}}\right)\right\} \delta x(t)\, dt + \text{higher order terms.} \tag{3.148}$$

Since we require that $\delta x(a) = \delta x(b) = 0$ in order to preserve the endpoints, the boundary terms vanish and we see that in order to make $\delta I = 0$ to first order, we require that

$$\int_a^b \left\{\frac{\partial F}{\partial x} - \frac{d}{dt}\left(\frac{\partial F}{\partial \dot{x}}\right)\right\} \delta x(t)\, dt = 0 \tag{3.149}$$

This integral must vanish for all permitted variations $\delta x(t)$ about the extreme solution $x(t)$. Since $\delta x(t)$ is arbitrary at all points within the interval (a, b), this can only happen if the integrand in braces vanishes for all t. i.e., if

$$\frac{\partial F}{\partial x} - \frac{d}{dt}\left(\frac{\partial F}{\partial \dot{x}}\right) = 0 \tag{3.150}$$

This partial differential equation is known as the **Euler-Lagrange equation** for the variational problem. In our problem,

$$F(t, x, \dot{x}) = \sqrt{1 + \dot{x}^2} \tag{3.151}$$

and so

$$\frac{\partial F}{\partial x} = 0 \text{ and } \frac{\partial F}{\partial \dot{x}} = \frac{\dot{x}}{\sqrt{1 + \dot{x}^2}} \tag{3.152}$$

The Euler-Lagrange equations for the problem thus read

$$\frac{d}{dt}\left(\frac{\dot{x}}{\sqrt{1 + \dot{x}^2}}\right) = 0 \text{ or that } \frac{\dot{x}}{\sqrt{1 + \dot{x}^2}} = \text{constant} \tag{3.153}$$

This can only happen if $\dot{x}$ is a constant, indicating that the curve of extremal length is indeed a straight line, as expected.

It should be noted that:

1. Minimizing a functional over a space of functions is like minimizing over an infinite number of variables. For each $t \in [a, b]$, we may think of the value of $x(t)$ as being a separate independent variable for the minimization problem. It is essentially the independence of the $\delta x(t)$ which allows us to conclude that the integrand in (3.149) must vanish at each point t.

2. The conditions $\delta x(a) = 0$ and $\delta x(b) = 0$ were important in the above derivation. Suppose we change the statement of the problem so that $\delta x(a) = 0$ is still required but $\delta x(b)$ is left arbitrary. In order to make $\delta I = 0$ in equation (3.148), it is still necessary to satisfy the Euler-Lagrange equation, but in addition, we must make the boundary term vanish as well.
$$\left[\delta x(t)\frac{\partial F}{\partial \dot{x}}(t)\right]_a^b = 0 \tag{3.154}$$
Since $\delta x(a) = 0$, the lower limit is zero. At b on the other hand, since $\delta x(b)$ is now arbitrary, we must insist that
$$\frac{\partial F}{\partial \dot{x}}(b) = 0 \tag{3.155}$$
For the minimum arc length problem, this means that
$$\frac{\dot{x}(b)}{\sqrt{1+\dot{x}(b)^2}} = 0 \tag{3.156}$$
or that $\dot{x}(b) = 0$. Combining this with the result from the Euler-Lagrange equation that $\dot{x}$ is constant, we see that $\dot{x} = 0$ over the whole interval and the curve degenerates to a horizontal straight line. This is because lifting the requirement that $\delta x(b) = 0$ means that although the curve is still constrained to pass through (a, c) since $\delta x(a) = 0$, the variation of the curve is arbitrary at b, and so the curve can take on any value there, i.e., it is no longer constrained to pass through (b, d). As a result the curve through (a, c) with the shortest length is found to be a horizontal straight line which goes through (b, c) rather than (b, d).

Exercise: Show that if we wish to minimize a functional of the form
$$I(x) = \int_a^b F\left(t, x, \dot{x}, \ddot{x}, x^{(3)}, ..., x^{(n)}\right) dt \tag{3.157}$$
where $x^{(k)}$ denotes the k'th derivative of x with respect to t subject to the conditions that $\delta x(a) = \delta x(b) = 0$, the function $x(t)$ must satisfy an Euler-Lagrange equation of the form
$$\frac{\partial F}{\partial x} - \frac{d}{dt}\left(\frac{\partial F}{\partial \dot{x}}\right) + \frac{d^2}{dt^2}\left(\frac{\partial F}{\partial \ddot{x}}\right) - \frac{d^3}{dt^3}\left(\frac{\partial F}{\partial x^{(3)}}\right) + ... + (-1)^n \frac{d^n}{dt^n}\left(\frac{\partial F}{\partial x^{(n)}}\right) = 0 \tag{3.158}$$

3.8.3 Minimization of a functional involving a several functions

We now consider the action principle in the context of the calculus of variations. Here we have to find an extremum of
$$S(q_1, ..., q_s) = \int_{t_1}^{t_2} L(q_1, ..., q_s, \dot{q}_1, ..., \dot{q}_s, t)\ dt. \tag{3.159}$$
Since the initial configuration at t_1 and the final configuration at t_2 are specified, the variations must vanish at the endpoints, i.e., $\delta q_j(t_1) = 0$ and $\delta q_j(t_2) = 0$ for $j = 1, ..., s$. It is straightforward to extend the considerations of the previous section to show that in this case, the variation of S vanishes to first order if we satisfy the s Euler-Lagrange equations
$$\frac{\partial L}{\partial q_j} - \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}_j}\right) = 0 \tag{3.160}$$
for $j = 1, ..., s$. Thus we recover the Lagrange equations of motion (and Newton's laws of motion) from the action principle.

3.9 Lagrange Multipliers and Constraints

When solving problems which involve finding the **constrained** extremum of a function, the method of Lagrange multipliers is often useful. Recall that for constrained optimization over a finite dimensional space, we can find the optimum of $V(q_1,...,q_s)$ subject to the k constraints $G_1(q_1,...,q_s)=0,...,G_k(q_1,...,q_s)=0$ by considering the **unconstrained** optimization of the auxiliary function

$$U(q_1,...,q_s)=V(q_1,...,q_s)+\lambda_1 G_1(q_1,...,q_s)+...+\lambda_k G_k(q_1,...,q_s) \tag{3.161}$$

where $\lambda_1,...,\lambda_k$ are called Lagrange multipliers. This unconstrained optimization problem gives s equations for the vanishing partial derivatives: $\partial U/\partial q_j=0$ for $j=1,...,s$. The k Lagrange multipliers are determined by requiring that the solution satisfy the s equations of constraint.

It should be noted that there is one Lagrange multiplier for each constraint in the problem. When the technique is applied to the calculus of variations, so that a function satisfying one or more constraints is required, essentially the same procedure is followed, except that care is required in order to count correctly the number of constraints and consequently the number of Lagrange multipliers that are required. If a constraint involves an integral over the entire interval or the value of the function at one point, this is only one constraint, and so a single Lagrange multiplier is needed, which is a constant. On the other hand, if the constraint involves the function obeying some relationship at every point within an interval, this is effectively an infinite continuum of constraints, one for each point within the interval at which the constraint is satisfied. The infinite number of Lagrange multipliers required to impose such a constraint may be regarded as a Lagrange multiplier function $\lambda(t)$ defined on the interval within which the constraints are satisfied.

As an example of a situation in which a single Lagrange multiplier is required, we consider the problem of minimizing the arc length of a curve passing through two endpoints as before, but with the additional condition that the area under the curve is now equal to some prescribed value. This is related to the isoperimetric problem attributed to Queen Dido of Carthage which seeks to maximize the area enclosed by a plane curve with a specified perimeter. The solution is known to be a circle, as we may confirm by using the method of Lagrange multipliers:

In this problem we seek to find extremum of

$$I(x)=\int_a^b F(t,x,\dot{x})\,dt \text{ where } F(t,x,\dot{x})=\sqrt{1+\dot{x}^2} \tag{3.162}$$

subject to the constraint that

$$\int_a^b x(t)\,dt=A \tag{3.163}$$

for some specified area A. Since this is a single constraint, the method of Lagrange multipliers requires us to consider

$$\begin{aligned} J(x) &= \int_a^b F(t,x,\dot{x})\,dt+\lambda\left(\int_a^b x\,dt-A\right) && (3.164)\\ &= \int_a^b \left(\sqrt{1+\dot{x}^2}+\lambda x\right)dt-\lambda A && (3.165)\end{aligned}$$

for which the Euler-Lagrange equation is

$$\frac{\partial}{\partial x}\left(\sqrt{1+\dot{x}^2}+\lambda x\right)-\frac{d}{dt}\frac{\partial}{\partial \dot{x}}\left(\sqrt{1+\dot{x}^2}+\lambda x\right)=0 \tag{3.166}$$

or

$$\lambda-\frac{d}{dt}\left(\frac{\dot{x}}{\sqrt{1+\dot{x}^2}}\right)=0 \tag{3.167}$$

This may be integrated to yield

$$\frac{\dot{x}}{\sqrt{1+\dot{x}^2}}=\lambda t+c \tag{3.168}$$

or

$$\dot{x} = \frac{\lambda t + c}{\sqrt{1 + (\lambda t + c)^2}} \tag{3.169}$$

which may be integrated again to yield

$$(x - d)^2 + \left(t + c\lambda^{-1}\right)^2 = \lambda^{-2}. \tag{3.170}$$

This is the equation of a circle.

As an example when the Lagrange multiplier is really a function as it imposes constraints at each point within an interval, we consider the problem of differential constraints in the next section.

3.10 Differential Constraints in the Variational Framework

As mentioned previously, a mechanical system is constrained if the space of permitted configurations is limited in some way. **Holonomic constraints** are those in which the restrictions on the configurations are expressible as equality conditions on the coordinate functions. All other constraints are non-holonomic. As an example of a non-holonomic constraint, consider describing the motion of a particle constrained to move on or above the surface of a sphere of radius R centred on the origin. Its Cartesian coordinates satisfy

$$x^2 + y^2 + z^2 \geq R^2 \tag{3.171}$$

which is an inequality constraint. Other non-holonomic constraints may take the form of differential constraints which relate small changes in the coordinate values, such as occur in problems involving rolling without slipping. All holonomic constraints and some non-holonomic constraints may be written in **differential form** showing variations which are consistent with the constraints.

Consider as an example a pendulum of length l for which the coordinates (x, y, z) of the bob satisfy the condition $x^2 + y^2 + z^2 = l^2$. If we displace the bob from a valid position (x, y, z) by $(\delta x, \delta y, \delta z)$, the resulting configuration is valid provided that

$$(x + \delta x)^2 + (y + \delta y)^2 + (z + \delta z)^2 = l^2 \tag{3.172}$$

To first order, this means that the variations satify

$$x\,\delta x + y\,\delta y\, + z\,\delta z = 0. \tag{3.173}$$

More generally, if we have a holonomic constraint of the form

$$G\left(q_1, q_2, ..., q_M\right) = 0, \tag{3.174}$$

the requirement that $(\delta q_1, ..., \delta q_M)$ satisfy

$$G\left(q_1 + \delta q_1, q_2 + \delta q_2, ..., q_M + \delta q_M\right) = 0 \tag{3.175}$$

can be written in differential form as the constraint

$$\left(\frac{\partial G}{\partial q_1}\right) \delta q_1 + ... + \left(\frac{\partial G}{\partial q_M}\right) \delta q_M = 0. \tag{3.176}$$

Rolling constraints which may be non-holonomic may often be written in differential form. For example, the rolling constraint for a wheel of radius a whose axle is horizontal and whose centre is above the point (x, y) in the horizontal plane may be written as the two differential constraints

$$\delta x = a\,\delta\theta\,\sin\psi \tag{3.177}$$
$$\delta y = a\,\delta\theta\,\cos\psi \tag{3.178}$$

where θ is the angle through which the wheel rotates and ψ is an angle indicating the direction in which the axle of the wheel.

Differential constraints may be incorporated into the action principle by using Lagrange multipliers. A differential constraint is a statement which specifies what variations of the trajectory are permitted in order that the varied path still satisfy the constraint and thus needs to be included into the extremum problem for the action.

It is important to remember that a differential constraint such as $x\,\delta x+y\,\delta y+z\,\delta z=0$ is actually a continuum of constraints since it means that for **all** t in the interval,

$$x(t)\ \delta x(t)+y(t)\ \delta y(t)\ +z(t)\ \delta z(t)=0. \tag{3.179}$$

In order to impose such a constraint, we need a Lagrange multiplier function $\lambda(t)$.

Example: Consider the problem of a circular cylinder of radius a, mass m and moment of inertia I about its axis rolling down an inclined plane making an angle ϕ with the horizintal. If the cylinder does not slip, the position of the cylinder down the slope s is related to the angle of rotation of the cylinder by the differential relation $\delta s=a\,\delta\theta$. The action principle requires that we find the extremum of

$$S(s,\theta)=\int_{t_1}^{t_2}\left[\frac{1}{2}\left(m\dot{s}^2+I\dot{\theta}^2\right)+mgs\sin\phi\right]dt \tag{3.180}$$

subject to the constraint that the variations satisfy $\delta s-a\,\delta\theta=0$ at all $t\in[t_1,t_2]$. If we vary s by δs and θ by $\delta\theta$, the variation in the action may be written using the variational principle argument as

$$\delta S=\int_{t_1}^{t_2}\left(\left\{-\frac{d}{dt}\left(\frac{\partial L}{\partial\dot{s}}\right)+\frac{\partial L}{\partial s}\right\}\delta s+\left\{-\frac{d}{dt}\left(\frac{\partial L}{\partial\dot{\theta}}\right)+\frac{\partial L}{\partial\theta}\right\}\delta\theta\right)dt \tag{3.181}$$

We now include the constraint via a Lagrange multiplier **function** $\lambda(t)$. We consider extremum of $J(s,\theta)$ where

$$\begin{aligned}\delta J &= \delta S+\int_{t_1}^{t_2}\lambda(t)\left(\delta s-a\,\delta\theta\right)\,dt & (3.182)\\ &= \int_{t_1}^{t_2}\left(\left\{-\frac{d}{dt}\left(\frac{\partial L}{\partial\dot{s}}\right)+\frac{\partial L}{\partial s}+\lambda(t)\right\}\delta s+\left\{-\frac{d}{dt}\left(\frac{\partial L}{\partial\dot{\theta}}\right)+\frac{\partial L}{\partial\theta}-a\lambda(t)\right\}\delta\theta\right)dt & (3.183)\end{aligned}$$

Now we can treat the problem as unconstrained, and consider the variations δs and δt as being independent. Setting the factors in braces to zero yields

$$\begin{aligned}\frac{d}{dt}\left(\frac{\partial L}{\partial\dot{s}}\right)-\frac{\partial L}{\partial s} &= \lambda(t) & (3.184)\\ \frac{d}{dt}\left(\frac{\partial L}{\partial\dot{\theta}}\right)-\frac{\partial L}{\partial\theta} &= -a\lambda(t) & (3.185)\end{aligned}$$

which in the example problem reduces to

$$\begin{aligned}m\ddot{s}-mg\sin\theta &= \lambda(t) & (3.186)\\ I\ddot{\theta} &= -a\lambda(t) & (3.187)\end{aligned}$$

Solving these together with the constraint equation, which is implies that $\ddot{s}=a\ddot{\theta}$, yields

$$\ddot{s}=\frac{mg\sin\phi}{m+I/a^2} \tag{3.188}$$

and

$$\lambda(t)=-\frac{I\ddot{\theta}}{a}=-\frac{I}{a^2}\left(\frac{mg\sin\phi}{m+I/a^2}\right). \tag{3.189}$$

Notice that λ gives the force of constraint, since

$$\frac{d}{dt}\left(\frac{\partial T}{\partial\dot{s}}\right)-\frac{\partial T}{\partial s}=Q_s=-\frac{\partial V}{\partial s}+\lambda \tag{3.190}$$

Here Q_s denotes the total force on the cylinder acting down the slope. It is composed of two terms. The term $-\partial V/\partial s = mg\sin\phi$ is the component of the gravitaional force down the slope, while λ is the frictional force which keeps the cylinder from slipping. Note that this system is conservative despite the presence of friction, since the system does no work against the frictional force.

More generally, we can consider k simultaneous differential constraints of the form

$$a_{11}(q,t)\,\delta q_1 + \ldots + a_{1s}(q,t)\,\delta q_s = 0 \tag{3.191}$$

$$\vdots$$

$$a_{k1}(q,t)\,\delta q_1 + \ldots + a_{ks}(q,t)\,\delta q_s = 0 \tag{3.192}$$

where, as usual, q denotes $q_1,\ldots,q_s$. This requires k Lagrange multiplier functions $\lambda_1(t),\ldots,\lambda_k(t)$ and the action principle becomes

$$\delta S = \int_{t_1}^{t_2} \sum_{j=1}^{s} \left(-\frac{d}{dt}\frac{\partial L}{\partial \dot q_j} + \frac{\partial L}{\partial q_j} \right) \delta q_j \, dt = 0 \tag{3.193}$$

subject to the above constraints. We thus consider when

$$\int_{t_1}^{t_2} \sum_{j=1}^{s} \left(-\frac{d}{dt}\frac{\partial L}{\partial \dot q_j} + \frac{\partial L}{\partial q_j} + \sum_{l=1}^{k} a_{lj}\lambda_l(t) \right) \delta q_j \, dt = 0 \tag{3.194}$$

which leads to the Euler-Lagrange equations

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot q_j}\right) - \frac{\partial L}{\partial q_j} = \sum_{l=1}^{k} a_{lj}\lambda_l(t) \tag{3.195}$$

together with the k equations of constraint.

3.11 Hamiltonian Mechanics and the Canonical Equations

The Lagrange equations of motion are second order differential equations in the trajectories $q(t)$. In order to obtain a solution, it is necessary to specify both the positions $q_1,\ldots,q_s$ and the velocities $\dot q_1,\ldots,\dot q_s$ at an initial time. In the Hamiltonian formalism, instead of an s dimensional configuration space, we consider a $2s$ dimensional **phase space** whose coordinates are $q_1,\ldots,q_s$ and $p_1,\ldots,p_s$ where the p's denote the **conjugate momenta** defined by

$$p_j = \frac{\partial L}{\partial \dot q_j} \tag{3.196}$$

For Cartesian coordinates, p_j coincides with the usual mechanical momentum and for angular coordinates, p_j is usually (some component) of the angular momentum. It is possible to reformulate mechanics so as to arrive at equations for q and p which are **first-order** in time. This means that the future evolution of the system is determined by just the **values** of q and p at the initial time. A point is phase space thus acts as a complete description of the state of a mechanical system at a particular instant.

We wish to transform from a Lagrangian description, in which L is a function of q, $\dot q$ and t to one in which the fundamental mechanical quantity is a function of q, p and t. (Here, and in the following, q is a shorthand for $q_1,\ldots,q_s$ etc.) This may be achieved by a mathematical device known as the Legendre transformation which allows one to change variables without loss of information. The technique is also used in classical thermodynamics from which the following example is taken.

For a thermodynamical system with fixed particle number, it is known that all properties of the system may be derived once the energy E is known as a function of the volume V and the entropy S. This is because the fundamental thermodynamic relation states that

$$dE = TdS - PdV \tag{3.197}$$

which when compared with the usual expansion of the differential of E, namely

$$dE = \left(\frac{\partial E}{\partial S}\right) dS + \left(\frac{\partial E}{\partial v}\right) dV \tag{3.198}$$

allows us to identify

$$T = \left(\frac{\partial E}{\partial S}\right)_V \text{ and } P = -\left(\frac{\partial E}{\partial V}\right)_S. \tag{3.199}$$

From these relationships, other thermodynamic properties may be expressed in terms of the derivatives of E with respect to S and V. When considering systems at constant temperature, however, it is more convenient to consider T rather than S as an independent variable. In thermodynamics, this is done by defining a quantity known as the (Helmholtz) free energy

$$F = E - TS \tag{3.200}$$

which must then be rewritten as a function of T and of V alone. By making this definition, we see that

$$dF = dE - T\,dS - S\,dT \tag{3.201}$$

Using the fundamental relation for E, this leads to a fundamental relation for F

$$dF = -PdV - SdT \tag{3.202}$$

which indicates that if F is written in terms of V and of T, then

$$P = -\left(\frac{\partial F}{\partial V}\right)_T \text{ and } S = -\left(\frac{\partial F}{\partial T}\right)_V. \tag{3.203}$$

From $F(T,V)$ we can derive all thermodynamic quantities, just as we can from $E(S,V)$.

The key to the Legendre transform is the use of the product TS to effect the replacement of the variable S by the variable T. By defining the free energy as above, the term $T\,dS$ from the differential $d(TS)$ serves to remove the differential dS from the fundamental relation for E and replaces it with a differential $S\,dT$ involving the termperature.

In the case of mechanics, the **Hamiltonian** is defined as a function of q, p and t as

$$H(q,p,t) = p\dot{q} - L(q,\dot{q},t) \tag{3.204}$$

When evaluating H, the right-hand side must be rewritten in terms of q, p and t alone. With this definition,

$$dH = p\,d\dot{q} + \dot{q}\,dp - \frac{\partial L}{\partial q}dq - \frac{\partial L}{\partial \dot{q}}\,d\dot{q} - \frac{\partial L}{\partial t}\,dt. \tag{3.205}$$

By definition of p as $\partial L/\partial \dot{q}$, the dependence on the differential $d\dot{q}$ vanishes, and so

$$dH = \dot{q}\,dp - \frac{\partial L}{\partial q}dq - \frac{\partial L}{\partial t}\,dt. \tag{3.206}$$

Comparing this with

$$dH = \frac{\partial H}{\partial p}\,dp + \frac{\partial H}{\partial q}\,dq + \frac{\partial H}{\partial t}\,dt, \tag{3.207}$$

we see that

$$\frac{\partial H}{\partial p} = \dot{q} \tag{3.208}$$

$$\frac{\partial H}{\partial q} = -\frac{\partial L}{\partial q} = -\dot{p} \tag{3.209}$$

$$\frac{\partial H}{\partial t} = -\frac{\partial L}{\partial t} \tag{3.210}$$

where the Lagrange equations of motion are used to show that

$$\frac{\partial L}{\partial q} = \frac{d}{dt}\frac{\partial L}{\partial \dot{q}} = \dot{p}. \tag{3.211}$$

Similarly, if we have $L(q_1, ..., q_s, \dot{q}_1, ..., \dot{q}_s, t)$ we define

$$H(q_1, ..., q_s, p_1, ..., p_s, t) = \sum_{i=1}^{s} p_i \dot{q}_i - L \tag{3.212}$$

and we find that

$$\begin{aligned} \dot{q}_i &= \frac{\partial H}{\partial p_i} && (3.213)\\ \dot{p}_i &= -\frac{\partial H}{\partial q_i} && (3.214)\\ \frac{\partial H}{\partial t} &= -\frac{\partial L}{\partial t} && (3.215) \end{aligned}$$

which are known as Hamilton's canonical equations of motion. As promised, they are first order differential equations for the coordinates q, p of phase space.

Example: The simple pendulum in the Hamiltonian formalism

It is important to remember to write the Hamiltonian as a function of p_i, q_i and t, so that the velocities $\dot{q}_i$ do **not** appear. For the simple pendulum of length l, where θ, the angle from the vertical is the only generalized coordinate, the Lagrangian is

$$L = \frac{1}{2}ml^2\dot{\theta}^2 + mgl\cos\theta \tag{3.216}$$

and the momentum conjugate to θ is

$$p = \frac{\partial L}{\partial \dot{\theta}} = ml^2\dot{\theta} \tag{3.217}$$

By definition the Hamiltonian is

$$\begin{aligned} H &= p\dot{\theta} - L = ml^2\dot{\theta}^2 - \left(\frac{1}{2}ml^2\dot{\theta}^2 + mgl\cos\theta\right) && (3.218)\\ &= \frac{1}{2}ml^2\dot{\theta}^2 - mgl\cos\theta && (3.219) \end{aligned}$$

We must now use the definition of the momentum to eliminate the velocity $\dot{\theta}$. The result is

$$H = \frac{p^2}{2ml^2} - mgl\cos\theta. \tag{3.220}$$

Hamilton's canonical equations may be derived from this as

$$\begin{aligned} \dot{p} &= -\frac{\partial H}{\partial \theta} = -mgl\sin\theta && (3.221)\\ \dot{\theta} &= \frac{\partial H}{\partial p} = \frac{p}{ml^2} && (3.222) \end{aligned}$$

This gives two first-order differential equations for the motion of the point (θ, p) in the phase space. In phase space, a point corresponds to a state of the pendulum and with time, this state flows in accordance with the canonical equations. The flow lines do not cross in phase space, since there is only one motion possible, starting at a particular initial condition. The only points where flow lines may appear to cross are at critical points, where the system is at a position of stable or unstable equilibrium. The phase space of the simple pendulum (assuming that the length l remains fixed even when $|\theta|$ exceeds $\pi/2$) is shown in Figure 3.2. Note that the flow lines are traversed clockwise and are on the level surfaces of H if the Hamiltonian is a constant of the motion, as it is in this case.

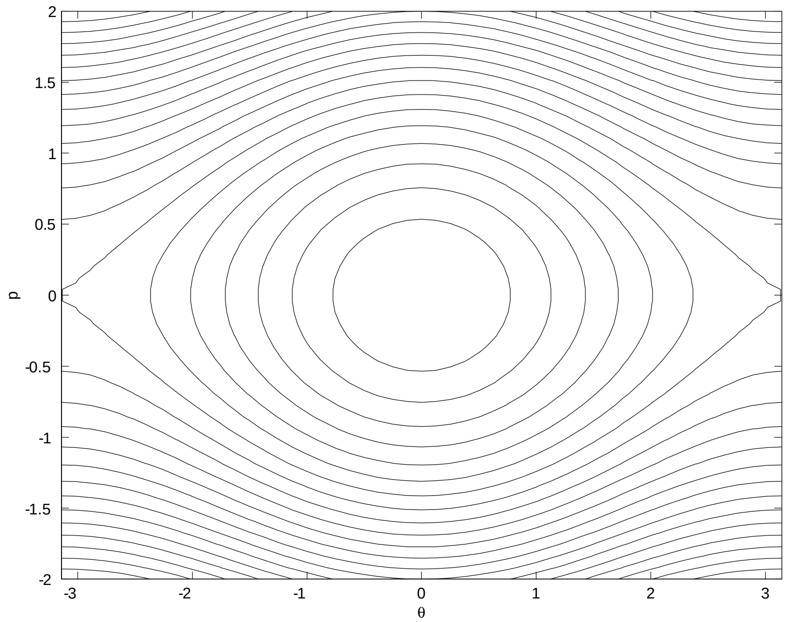

Figure 3.2 Phase plot for a simple pendulum

3.11.1 Physical Significance of the Hamiltonian

There are two main results:

1. If the system is conservative, i.e., if V depends only on the positions q_j and the time t, and if the coordinate transformations $x_i\left(q_1,...,q_s\right)$ from generalised coordinates to inertial Cartesian coordinates is **not** explicitly time-dependent, then the Hamiltonian is equal to the **total energy.**

   This may be proved by noting that if $x_i\left(q_1,...,q_s,\right)$ then

$$\dot{x}_i=\sum_{j=1}^{s}\frac{\partial x_i}{\partial q_j}\dot{q}_j \tag{3.223}$$

and so

$$\begin{aligned} T &= \sum_{i=1}^{3N}\frac{1}{2}m_i\dot{x}_i^2=\sum_{i=1}^{3N}\frac{1}{2}m_i\left(\sum_{j=1}^{s}\frac{\partial x_i}{\partial q_j}\dot{q}_j\right)^2 & (3.224)\\ &= \sum_{j=1}^{s}\sum_{k=1}^{s}\left(\sum_{i=1}^{3N}\frac{1}{2}m_i\frac{\partial x_i}{\partial q_j}\frac{\partial x_i}{\partial q_k}\right)\dot{q}_j\dot{q}_k & (3.225)\\ &= \sum_{j=1}^{s}\sum_{k=1}^{s}a_{jk}\left(q\right)\dot{q}_j\dot{q}_k & (3.226)\end{aligned}$$

where the a_{jk} are functions only of the $q_1,...,q_s$. Further, since V only depends on q and t,

$$\begin{aligned} p_i &= \frac{\partial L}{\partial \dot{q}_i}=\frac{\partial\left(T-V\right)}{\partial \dot{q}_i}=\frac{\partial T}{\partial \dot{q}_i} & (3.227)\\ &= \sum_{j=1}^{s}\sum_{k=1}^{s}a_{jk}\left(q\right)\frac{\partial}{\partial \dot{q}_i}\left(\dot{q}_j\dot{q}_k\right) & (3.228)\\ &= 2\sum_{j=1}^{s}a_{ij}\dot{q}_j & (3.229)\end{aligned}$$

since $a_{ik} = a_{ki}$. Substituting into the definition of the Hamiltonian yields

$$H = \sum_{i=1}^{s} p_i \dot{q}_i - L = 2\sum_{i=1}^{s}\sum_{j=1}^{s} a_{ij}\dot{q}_j\dot{q}_i - (T - V) = T + V \tag{3.230}$$

showing that H is the total energy. Note that:

(a) If the above conditions are fulfilled, H is the total energy, but it need not be a constant of the motion.

(b) The above conditions are sufficient but not necessary for H to be the total energy. In particular, for a moving charge in a constant electromagnetic field, we can show that $H = T + e\phi$, which is the total energy, although V is velocity-dependent

2. The condition for the Hamiltonian to be a **constant of the motion** is for H to be not explicitly dependent on t, since

$$\begin{aligned} \frac{dH}{dt} &= \sum_{i=1}^{s} \frac{\partial H}{\partial q_i}\dot{q}_i + \sum_{i=1}^{s} \frac{\partial H}{\partial p_i}\dot{p}_i + \frac{\partial H}{\partial t} \\ &= \sum_{i=1}^{s} (-\dot{p}_i)\,\dot{q}_i + \sum_{i=1}^{s} (\dot{q}_i)\,\dot{p}_i + \frac{\partial H}{\partial t} = \frac{\partial H}{\partial t}. \end{aligned}$$

The situation of greatest physical interest is when H is the total energy **and** H *is* constant on time. Sufficient conditions for this are if V depends on q_j alone (i.e., not on t) and the coordinate transformations from generalized coordinates to inertial Cartesian coordinates are not explicitly time-dependent.

3.12 Motion in Phase Space as a Flow

Let us define a vector $\boldsymbol{\xi}$ of $2s$ components consisting of the s positions followed by the s momenta. i.e., $\boldsymbol{\xi} = \begin{pmatrix} q \\ p \end{pmatrix}$. This is called the **state vector** of phase space. As the system state evolves, the state vector $\boldsymbol{\xi}$ moves in phase space. The derivative of $\boldsymbol{\xi}$ with respect to time is $\dot{\boldsymbol{\xi}} = \begin{pmatrix} \dot{q} \\ \dot{p} \end{pmatrix}$ which is known as the **phase velocity.** Let us consider a problem in which the Hamiltonian is time-independent so that we can write $H(\boldsymbol{\xi}) = H(q,p)$ instead of $H(q,p,t)$. The level surfaces of H form $2s-1$ dimensional hypersurfaces in phase space. The vector which is normal to the level surface of H has components $\partial H/\partial \xi_i$. The phase velocity vector is orthogonal to this since the inner product between them is

$$\sum_{i=1}^{2s} \dot{\boldsymbol{\xi}}_i \frac{\partial H}{\partial \xi_i} = \sum_{i=1}^{s}\left(\dot{q}_i \frac{\partial H}{\partial q_i} + \dot{p}_i \frac{\partial H}{\partial p_i}\right) = \sum_{i=1}^{s} \left[\dot{q}_i\,(-\dot{p}_i) + \dot{p}_i q_i\right] = 0. \tag{3.231}$$

This means that the phase velocity is at all times tangential to the level surfaces of H, as we would expect since the Hamiltonian is a constant of the motion.

At each point in phase space, there is a phase velocity which lies in the level surface of H. This may be thought of as describing the flow of a $2s$ dimensional "fluid" in phase space. Of course, a point within the fluid refers to an entire state of motion of the system of particles and a "volume" of fluid refers to a collection of neighbouring states. The main theorem regarding flows in phase space is that the flow is **incompressible**.

In ordinary space, a fluid is incompressible if its density remains constant in space and time. The equation of continuity applies to any fluid and relates the rate of change of the mass of fluid in a volume to the rate at which mass is transported through the boundary of the volume. If ρ is the density of the fluid, the mass of fluid in a volume V is given by

$$m = \int_V \rho\, dV \tag{3.232}$$

and the rate at which mass leaves the volume through the boundary $S = \partial V$ of V is

$$\int_{\partial V} \rho \mathbf{v} \cdot d\mathbf{S} \tag{3.233}$$

where $\mathbf{v}$ is the velocity vector of the fluid. The equation of continuity is thus

$$\frac{\partial}{\partial t} \int_V \rho \, dV = - \int_{\partial V} \rho \mathbf{v} \cdot d\mathbf{S} \tag{3.234}$$

Using the divergence theorem we see that the differential form of the equation of continuity is

$$\frac{\partial \rho}{\partial t} + \boldsymbol{\nabla} \cdot (\rho \mathbf{v}) = 0, \tag{3.235}$$

which may alternatively be written as

$$\frac{\partial \rho}{\partial t} + \mathbf{v} \cdot \boldsymbol{\nabla} \rho + \rho \, (\boldsymbol{\nabla} \cdot \mathbf{v}) = 0 \tag{3.236}$$

Now, if the density is to be constant, the first two terms vanish, and so $\boldsymbol{\nabla} \cdot \mathbf{v} = 0$. Similarly, if $\boldsymbol{\nabla} \cdot \mathbf{v} = 0$, the convective derivative of ρ vanishes and so ρ is constant. Thus a necessary and sufficient condition for incompressibility is that $\boldsymbol{\nabla} \cdot \mathbf{v} = \mathbf{0}$. In component form, this reads

$$\frac{\partial v_x}{\partial x} + \frac{\partial v_y}{\partial y} + \frac{\partial v_z}{\partial z} = 0 \tag{3.237}$$

or

$$\frac{\partial \dot{x}}{\partial x} + \frac{\partial \dot{y}}{\partial y} + \frac{\partial \dot{z}}{\partial z} = 0. \tag{3.238}$$

Generalizing this to the $2s$ dimensions of phase space, we describe a flow in phase space as incompressible iff

$$\sum_{i=1}^{2s} \frac{\partial \dot{\xi}_i}{\partial \xi_i} = 0 \tag{3.239}$$

We may write the sum more explicitly as a sum over the momenta and a sum over the positions. Thus

$$\sum_{i=1}^{2s} \frac{\partial \dot{\xi}_i}{\partial \xi_i} = \sum_{i=1}^{s} \left(\frac{\partial \dot{q}_i}{\partial q_i} + \frac{\partial \dot{p}_i}{\partial p_i} \right) \tag{3.240}$$

$$= \sum_{i=1}^{s} \left(\frac{\partial}{\partial q_i} \left(\frac{\partial H}{\partial p_i} \right) + \frac{\partial}{\partial p_i} \left(- \frac{\partial H}{\partial q_i} \right) \right) = 0 \tag{3.241}$$

where we have used Hamilton's canonical equations. Thus we see that the flow of points in phase space as the dynamics unfolds is indeed incompressible and the phase space "volume" of a set of adjacent initial conditions is preserved by the evolution. This is known as Liouville's theorem.

Despite Liouville's theorem, it is known that for many systems, the motion of points in phase space are very sensitive functions of the initial conditions. Thus, points in phase space which are initially close to each other often diverge rapidly under the evolution. This is the origin of the chaotic behaviour exhibited by many mechanical systems and means that even though the equations of motion are deterministic, they are not useful for making long-term predictions since even microscopically small uncertainties in the specification of the initial conditions can lead to large uncertainties in the predicted state after some time. This means that even though the volume occupied by the states does not change, it can get spread around the phase space in very complicated ways as the dynamics folds, stretches and otherwise distorts the volume. As an analogy, it may be useful to think of a small drop of ink added to a large volume of water. Even though the volume of ink does not change, it does eventually spread throughout the volume of water.

3.12.1 Poisson Brackets

It is possible to describe the flow of points in phase space in an elegant way by using a mathematical construction known as Poisson brackets. Let $F(q,p,t)$ denote some dynamical variable which depends on the state of the system in phase space. As we follow the motion of the system, the variation of F with time is given by

$$\frac{dF}{dt} = \sum_{i=1}^{s} \left(\frac{\partial F}{\partial q_i}\dot{q}_i + \frac{\partial F}{\partial p_i}\dot{p}_i \right) + \frac{\partial F}{\partial t} \tag{3.242}$$

According to Hamilton's canonical equations, we can write $\dot{q}_i$ and $\dot{p}_i$ in terms of derivatives of H. This yields

$$\frac{dF}{dt} = \sum_{i=1}^{s} \left(\frac{\partial F}{\partial q_i}\frac{\partial H}{\partial p_i} - \frac{\partial F}{\partial p_i}\frac{\partial H}{\partial q_i} \right) + \frac{\partial F}{\partial t} \tag{3.243}$$

The sum involving derivatives of F and H turns out to be an extremely important quantity, called the Poisson bracket of F and H, and written as $[F,H]$. For any two dynamical variables, A and B, the Poisson bracket of A and B is defined by

$$[A,B] = \sum_{i=1}^{s} \left(\frac{\partial A}{\partial q_i}\frac{\partial B}{\partial p_i} - \frac{\partial A}{\partial p_i}\frac{\partial B}{\partial q_i} \right) \tag{3.244}$$

where (q,p) are a set of canonically conjugate variables. Note that for any dynamical variable $[A,A] = 0$ and that for any pair of variables, $[A,B] = -[B,A]$. Even though $[A,B]$ is defined with respect to a particular set of canonical coordinates (q,p), it can be shown that its value is unchanged if we use a different coordinate description of phase space.

The total time derivative of F may thus be written as

$$\frac{dF}{dt} = [F,H] + \frac{\partial F}{\partial t}, \tag{3.245}$$

and in particular, the Hamilton's canonical equations may be rewritten as

$$\dot{q}_i = [q_i, H] \text{ and } \dot{p}_i = [p_i, H] \tag{3.246}$$

since q_i and p_i are not explicitly dependent on time. On the other hand, if we set $F = H$ in equation (3.245), we find that

$$\frac{dH}{dt} = \frac{\partial H}{\partial t} \tag{3.247}$$

since $[H,H] = 0$. Thus we see that H is a constant of the motion if it is not explictly time-dependent. The similarity of (3.245) to the Heisenberg equations of motion in quantum mechanics should be apparent. In quantum mechanics, the Poisson bracket is replaced by the commutator divided by $i\hbar$, so that the Heisenberg equation of motion for an operator F is

$$\frac{dF}{dt} = \frac{1}{i\hbar}[F,H] + \frac{\partial F}{\partial t} \tag{3.248}$$

The correspondence between Poisson brackets and the commutator brackets of quantum mechanics is quite profound. In particular, it is easy to check that for Poisson brackets,

$$[q_j, q_k] = 0, \ [p_j, p_k] = 0 \text{ and } [q_j, p_k] = \delta_{jk} \tag{3.249}$$

while for commutator brackets the corresponding relationships are

$$[q_j, q_k] = 0, \ [p_j, p_k] = 0 \text{ and } [q_j, p_k] = i\hbar\delta_{jk} \tag{3.250}$$

For both Poisson brackets and commutator brackets, we have the identities

$$[AB, C] = A[B,C] + [A,C]B \tag{3.251}$$

$$[A, BC] = B[A,C] + [A,B]C \tag{3.252}$$

It is then easy to see that for Poisson brackets,

$$[q_j, p_k^n] = np_k^{n-1}\delta_{jk} \tag{3.253}$$

$$\left[q_j^n, p_k\right] = nq_j^{n-1}\delta_{jk} \tag{3.254}$$

so that for any function $F(q,p)$,

$$[q_j, F(q,p)] = \frac{\partial F}{\partial p_j} \tag{3.255}$$

and

$$[F(q,p), p_k] = \frac{\partial F}{\partial q_k} \tag{3.256}$$

Applying these to the components of the angular momentum for a single particle, where $J_x = yp_z - zp_y$ *et cyc.,* we find the relations

$$[J_x, J_y] = J_z,\ [J_y, J_z] = J_x \text{ and } [J_z, J_x] = J_y \tag{3.257}$$

These may be compared with the corresponding commutator relations in quantum mechanics

$$[J_x, J_y] = i\hbar J_z,\ [J_y, J_z] = i\hbar J_x \text{ and } [J_z, J_x] = i\hbar J_y \tag{3.258}$$

It is found that if a system can be described in classical mechanics using Poisson brackets, the quantum mechanical equations of motion may be formed simply by replacing dynamical variables by quantum mechanical observables and replacing the Poisson brackets with the commutator divided by $i\hbar$.

3.13 Canonical Transformations

The dynamics of a mechanical system may be described in terms of the trajectories which it executes in phase space. If there are s degrees of freedom, there are $2s$ phase-space coordinates, forming s conjugate pairs satisfying the Hamilton canonical equations of motion. Motion may be thought of as a flow in phase space, which as we have seen previously, is incompressible. In this section, we consider ways of changing coordinates in phase space in an attempt to simplify the flow. Such transformations are known as canonical or contact transformations.

When do two sets of phase space coordinates (q_i, p_i) and (Q_i, P_i) describe the same dynamics? If we express a particular system trajectory which starts at time t_1 and ends at time t_2 in the two coordinate systems, the actions along the paths do not need to be the same. It is only necessary that if the trajectory is perturbed in some way (while preserving the endpoints), the **variations** of the actions should coincide. In this way, the paths of extremal action will represent the same motion in the two coordinate systems, and Hamilton's canonical equations will hold for both coordinate descriptions.

Let $H(q,p,t)$ and $H'(Q,P,t)$ denote the Hamiltonians for the two coordinate systems. As we shall see, it is not even necessary that H' coincide with H at the corresponding point in phase space. Note that q is shorthand for $q_1, ..., q_s$ and p for $p_1, ..., p_s$. The action for a path in the interval $[t_1, t_2]$ is given by

$$S(q,p) = \int_{t_1}^{t_2} \left(\sum_{i=1}^{s} p_i \dot{q}_i - H(q,p,t) \right) dt, \tag{3.259}$$

when the phase space is described using coordinates $(q,p) \equiv (q_1, ..., q_s, p_1, ..., p_s)$ or by

$$S'(Q,P) = \int_{t_1}^{t_2} \left(\sum_{i=1}^{s} P_i \dot{Q}_i - H'(Q,P,t) \right) dt, \tag{3.260}$$

when the phase space is described using coordinates $(Q,P) \equiv (Q_1, ..., Q_s, P_1, ..., P_s)$. We want the **variations** δS and $\delta S'$ to coincide for the same variation in the trajectories. One way of ensuring this is for the integrands to be equal, but this is not in fact necessary. To see this, let us suppose that $F(q,Q,t)$ is an arbitrary function of q, Q and t. Since the variations of the trajectory vanish at the endpoints, we see that for any valid variation,

$$\delta\left[F\left(q\left(t_2\right),Q\left(t_2\right),t_2\right)-F\left(q\left(t_1\right),Q\left(t_1\right),t_1\right)\right]=0 \tag{3.261}$$

or

$$\delta\int_{t_1}^{t_2}\frac{dF}{dt}\,dt=0 \tag{3.262}$$

If all we want is $\delta S-\delta S'=0$, we can achieve this even if

$$\delta\int_{t_1}^{t_2}\left(\sum_{i=1}^{s}p_i\dot{q}_i-H\left(q,p,t\right)\right)dt-\delta\int_{t_1}^{t_2}\left(\sum_{i=1}^{s}P_i\dot{Q}_i-H'\left(Q,P,t\right)\right)dt=\delta\int_{t_1}^{t_2}\frac{dF}{dt}\,dt \tag{3.263}$$

since the right-hand side is zero. The total derivative of $F\left(q\left(t\right),Q\left(t\right),t\right)$ is given by

$$\frac{dF}{dt}=\sum_{i=1}^{s}\left(\frac{\partial F}{\partial q_i}\dot{q}_i+\frac{\partial F}{\partial Q_i}\dot{Q}_i\right)+\frac{\partial F}{\partial t}, \tag{3.264}$$

and so we get equality of the variations if

$$\delta\int_{t_1}^{t_2}\left\{\sum_{i=1}^{s}\left[\left(p_i-\frac{\partial F}{\partial q_i}\right)\dot{q}_i-\left(P_i+\frac{\partial F}{\partial Q_i}\right)\dot{Q}_i\right]+\left(H'-H-\frac{\partial F}{\partial t}\right)\right\}dt=0. \tag{3.265}$$

Thus, if we set

$$p_i = \frac{\partial F}{\partial q_i}, \tag{3.266}$$

$$P_i = -\frac{\partial F}{\partial Q_i}, \tag{3.267}$$

$$\text{and } H' = H+\frac{\partial F}{\partial t}, \tag{3.268}$$

the variations in the actions will coincide and Hamilton's canonical equations will describe the same motion in the two coordinate systems. The function $F(q,Q,t)$ is called the **generating function** of the canonical transformation.

Example 1: It is important to realize that the above derivation shows that for each choice of F, we get a novel coordinate description of phase space in terms of s pairs of canonically conjugate variables. Thus there is considerable freedom in describing the phase space of any motion. As an example, consider the motion of a particle under gravity. If q and p are the vertical position and momentum respectively of a mass m, the Hamiltonian is

$$H=\frac{p^2}{2m}+mgq \tag{3.269}$$

and the canonical equations of motion are

$$\dot{q}=\frac{\partial H}{\partial p}=\frac{p}{m}\text{ and }\dot{p}=-\frac{\partial H}{\partial q}=-mg. \tag{3.270}$$

Let us arbitrarily choose F to be some function of q, Q and t. For a start, suppose we use a time-independent generating function

$$F=qQ^2 \tag{3.271}$$

Then the equations of transformation (3.266–3.267) are

$$p = \frac{\partial F}{\partial q}=Q^2 \tag{3.272}$$

$$P = -\frac{\partial F}{\partial Q}=-2qQ \tag{3.273}$$

We may use these to write the new coordinates in terms of the old and vice versa. We find that

$$p = Q^2 \text{ and } q = -\frac{P}{2Q} \tag{3.274}$$

and

$$P = -2qp^{1/2} \text{ and } Q = p^{1/2} \tag{3.275}$$

Since F is time independent, equation (3.268) reads $H' = H$. This means that in order to find H', we simply express H in terms of the new coordinates. Using (3.269) and (3.274),

$$H' = \frac{Q^4}{2m} - \frac{mgP}{2Q} \tag{3.276}$$

If the derivation is correct, Hamilton's canonical equations for this Hamiltonian describes the same motion (i.e. the particle falling under gravity) in the new phase space coordinates P and Q. They are

$$\dot{Q} = \frac{\partial H'}{\partial P} = -\frac{mg}{2Q} \tag{3.277}$$

$$\dot{P} = -\frac{\partial H'}{\partial Q} = -\frac{2Q^3}{m} + \frac{mgP}{2Q^2} \tag{3.278}$$

It is easy to check that these are consistent with the original equations of motion (3.270) by using the transformation equations (3.274) and (3.275). We see that

$$\dot{q} = -\frac{d}{dt}\left(\frac{P}{2Q}\right) = -\frac{Q\dot{P} - P\dot{Q}}{2Q^2} = -\frac{Q\left(-\frac{2Q^3}{m} + \frac{mgP}{2Q^2}\right) - P\left(\frac{mg}{2Q}\right)}{2Q^2} = \frac{Q^2}{m} = \frac{p}{m} \tag{3.279}$$

and

$$\dot{p} = 2Q\dot{Q} = 2Q\left(-\frac{mg}{2Q}\right) = -mg \tag{3.280}$$

as expected. Note also that the transformation specified by (3.274) and (3.275) is canonical for every Hamiltonian describing a system with one degree of freedom, so we could have applied the same transformation to a simple harmonic oscillator, a simple pendulum etc.

Example 2 In this example, let us consider a generating function which is explicitly time-dependent, such as

$$F = Qqt \tag{3.281}$$

In this case the transformation equations are also explicitly time dependent:

$$p = \frac{\partial F}{\partial q} = Qt, \tag{3.282}$$

$$P = -\frac{\partial F}{\partial Q} = -qt, \tag{3.283}$$

$$H' = H + \frac{\partial F}{\partial t} = H + Qq. \tag{3.284}$$

These may be written in explicit form as

$$p = Qt \text{ and } q = -\frac{P}{t} \tag{3.285}$$

and

$$P = -qt \text{ and } Q = \frac{p}{t} \tag{3.286}$$

The novel feature is the third transformation equation which shows that H' and H do not take on the same values at corresponding points in phase space. For the particle falling under gravity,

$$H' = \frac{p^2}{2m} + mgq + Qq, \tag{3.287}$$

which must be rewritten in terms of Q, P and t to give

$$H' = \frac{(Qt)^2}{2m} + mg\left(-\frac{P}{t}\right) + Q\left(-\frac{P}{t}\right) = \frac{Q^2t^3 - 2m^2gP - 2QPm}{2mt} \tag{3.288}$$

The canonical equations for this Hamiltonian are

$$\dot{Q} = \frac{\partial H'}{\partial P} = -\frac{mg+Q}{t} \tag{3.289}$$

$$\dot{P} = -\frac{\partial H'}{\partial Q} = \frac{P}{t} - \frac{Qt^2}{m} \tag{3.290}$$

It is easy to check that these are consistent with the original equations of motion.

3.13.1 Alternative Forms of the Transformation Equations

So far, we have considered a generating functions which are functions of q, Q and t, i.e., on the old coordinates, the new coordinates and time. For each such generating function, we obtain a canonical transformation between phase space coordinates. It turns out to be possible to start with functions of other variables and still generate canonical transformations. In particular, we can use generating functions which depend on q, P and t, or on p, Q and t or on p, P and t. In each case, the arguments are s old phase space variables, s new phase space variables and time. As an illustration, let us consider a generating function $G(q, P, t)$. We reduce the problem to the previous case by using a Legendre transformation. Starting with $F(q, Q, t)$ we see that

$$dF = \sum_{i=1}^{s}\left(\frac{\partial F}{\partial q_i}\,dq_i + \frac{\partial F}{\partial Q_i}\,dQ_i\right) + \frac{\partial F}{\partial t}\,dt \tag{3.291}$$

$$= \sum_{i=1}^{s}(p_i\,dq_i - P_i\,dQ_i) + (H' - H)\,dt. \tag{3.292}$$

where we have used (3.266–3.268). If we define

$$G = F + \sum_{i-1}^{s} P_iQ_i, \tag{3.293}$$

which is the Legendre transformation which replaces Q_i by P_i, then

$$dG = dF + \sum_{i-1}^{s}(P_i\,dQ_i + Q_i\,dP_i) \tag{3.294}$$

$$= \sum_{i=1}^{s}(p_i\,dq_i + Q_i\,dP_i) + (H' - H)\,dt \tag{3.295}$$

Reading off the coefficients of dq_i, dP_i and dt as the partial derivatives of G, we see that

$$p_i = \frac{\partial G}{\partial q_i} \tag{3.296}$$

$$Q_i = \frac{\partial G}{\partial P_i} \tag{3.297}$$

$$H' = H + \frac{\partial G}{\partial t} \tag{3.298}$$

Starting with any generating function $G(q, P, t)$, we can use these equations to find a canonical transformation for the phase space. Note that for the specific choice

$$G(q, P, t) = \sum_{i=1}^{s} q_iP_i, \tag{3.299}$$

the canonical transformation is the identity, i.e., $Q_i = q_i$ and $P_i = p_i$.

3.14 Hamilton-Jacobi Theory

We now consider choosing canonical transformations in such a way as to simplify the dynamical flow in phase space. Starting from a coordinate system (q, p) and a Hamiltonian $H(q, p)$ which is time independent, we shall see that we may transform to a new coordinate representation of phase space (Q, P) using a time-independent canonical transformation in such a way that the new Hamiltonian $H'(Q, P)$ is in fact independent of all the $\{Q_i\}_{i=1}^{s}$. This means that all the Q's are cyclic or ignorable coordinates, and consequently that all the P's are constants of the motion. This means that the P's depend only on the initial conditions and that for all time, $P_i(t) = P_i(0) \equiv \alpha_i$, say. The canonical equations of motion for the Q's are

$$\dot{Q}_i = \frac{\partial H'}{\partial P_i}. \tag{3.300}$$

Let us consider what the derivative on the right-hand side involves. Since H' is in fact independent of the Q's, it can depend only on the P's. By assumption, H' is not an explicit function of the time t. Since all the P's are constants of the motion, $\partial H'/\partial P_i$ must also be a constant of the motion, which may depend on the s initial conditions $\alpha = (\alpha_1, ..., \alpha_s)$. Let us write $\omega_i \equiv \partial H'/\partial P_i$, where ω_i is to be thought of as a function of the initial conditions α. It is now trivial to integrate the canonical equations for Q:

$$\dot{Q}_i = \frac{\partial H'}{\partial P_i} = \omega_i \Longrightarrow Q_i(t) = \omega_i t + \beta_i \tag{3.301}$$

where $\beta = (\beta_1, ..., \beta_s)$ are the s constants of integration which also depend on the initial conditions. In total, we have $2s$ initial conditions α, β which is as expected for a dynamical system with s degrees of freedom.

What this says is that for a system with a time-independent Hamiltonian, it is possible to find a time-independent canonical transformation such that the phase space flow becomes rather simple. An initial point (Q, P) simply "streams" parallel to each of the Q axes since the P coordinates remain constant. The phase velocity of the streaming is constant in time, and is just ω_i along the i'th direction. In effect, we have exchanged the complexity of the motion for the complexity of the phase-space coordinate transformation, but it is of interest to note that this can be done even though the canonical transformation is time-independent.

More generally, if the Hamiltonian is no longer assumed to be time-independent, $H(q, p, t)$, it turns out that it is possible to find a time-dependent canonical transformation such that in the new coordinate system, the new Hamiltonial $H'(Q, P)$ is identically zero! According to the canonical equations of motion, this means that $\dot{Q}_i = 0$ and $\dot{P}_i = 0$ so that all flow in phase space is brought to a stop by the canonical transformation. Of course, this does not mean that the physical system does not move, since the time-varying coordinate transformation in phase space means that a point with constant coordinates Q and P actually corresponds to time-varying coordinates and momenta q and p. In the new phase space coordinates (Q, P), a dynamical state of the system always has a "label" which does not change in time, and which is given by the initial conditions.

3.14.1 Time-dependent Hamiltonians

Suppose that we have a (possibly time-dependent) Hamiltonian $H(q, p, t)$. Using a time-dependent generating function of the form $G(q, P, t)$ and the transformation equations (3.296–3.298), we wish to make $H' = 0$. Using (3.298), this means that

$$0 = H' = H(q, p, t) + \frac{\partial G}{\partial t}(q, P, t). \tag{3.302}$$

We want this to be a way of finding the generating function $G(q, P, t)$ and so want to express p in terms of the independent variables (q, P, t). This can be done using (3.296), so that

$$\frac{\partial G}{\partial t}(q, P, t) + H\left(q, \frac{\partial G}{\partial q}, t\right) = 0. \tag{3.303}$$

When written out in full, this is

$$\frac{\partial G}{\partial t} + H\left(q_1, ..., q_s, \frac{\partial G}{\partial q_1}, ..., \frac{\partial G}{\partial q_s}, t\right) = 0 \tag{3.304}$$

which is seen to be a partial differential equation involving $s+1$ first-order derivatives of G. From this differential equation, which is known as the (time-dependent) Hamilton-Jacobi equation, we can find the dependence of G on t and on $q_1, ..., q_s$. There are going to be $s+1$ constants of integration, one of which may be removed since it is a trivial additive constant which does not affect the equations of transformation (3.296–3.298). The remaining s constants of integration may be taken to be the components of P. Exactly how this is done is not important, since **any** $G(q, P, t)$ which satisfies the Hamilton-Jacobi equation will give a valid canonical transformation for which the new Hamiltonian $H' = 0$. Of course, it is sometimes instructive to choose the constants of integration to be quantities having physical significance, such as the total energy.

Before proceeding to an example of finding the generating function in a specific situation, let us see if we can associate a meaning with $G(q, P, t)$. If we take the total derivative of G with respect to time along a trajectory,

$$\frac{dG}{dt} = \sum_{i=1}^{s}\left(\frac{\partial G}{\partial q_i}\dot{q}_i + \frac{\partial G}{\partial P_i}\dot{P}_i\right) + \frac{\partial G}{\partial t} \tag{3.305}$$

Since P_i are constants of the motion, the second terms in the sum vanish. Using the Hamilton-Jacobi equation for $\partial G/\partial t$, we see that

$$\frac{dG}{dt} = \sum_{i=1}^{s}\frac{\partial G}{\partial q_i}\dot{q}_i - H\left(q_1, ..., q_s, \frac{\partial G}{\partial q_1}, ..., \frac{\partial G}{\partial q_s}, t\right) \tag{3.306}$$

But using (3.296), we can identify $\partial G/\partial q_i$ as p_i. Thus,

$$\frac{dG}{dt} = \sum_{i=1}^{s} p_i\dot{q}_i - H(q, p, t) = L, \tag{3.307}$$

where L denotes the Lagrangian. Thus, the total time derivative of the generating function G along trajectories in phase space is precisely equal to the Lagrangian. Since we earlier defined the action S along a dynamical trajectory in phase space as the time-integral of L along that trajectory, we see that G is function from which the action along any dynamical trajectory in phase space may be found. If $\boldsymbol{\xi}_1 = (q, p, t_1)$ and $\boldsymbol{\xi}_2 = (q', p', t_2)$ are two points in phase space which are connected by a dynamical trajectory, the action S along that trajectory is just $G(\boldsymbol{\xi}_2) - G(\boldsymbol{\xi}_1)$. In practice, calculating the action this way is at least as difficult as solving the equations of motion and carrying out the time-integral of the Lagrangian, since we cannot in fact compute G until we know P as a function of q and p, which effectively requires a solution of the equations of motion. Nevertheless, this allows us to identify the generation function G with the action, (or more properly, Hamilton's first principal function) and so the Hamilton-Jacobi equations are often written as

$$\frac{\partial S}{\partial t} + H\left(q_1, ..., q_s, \frac{\partial S}{\partial q_1}, ..., \frac{\partial S}{\partial q_s}, t\right) = 0 \tag{3.308}$$

The action is thus revealed as not only being the quantity which takes on an extreme value along a dynamical trajectory (Hamilton's principle) but is also the generating function for the canonical transformation that brings flow in phase space to a stop.

Example: Let us solve the Hamilton-Jacobi equation for the special case of a simple harmonic oscillator. Note that the Hamilton for this example is in fact time-independent, but it is still necessary to use a time-dependent generating function in order to "stop" the flow. In one dimension, we have

$$H(q, p, t) = \frac{p^2}{2m} + \frac{1}{2}kq^2 \tag{3.309}$$

and so the Hamilton-Jacobi equation is

$$\frac{\partial S}{\partial t} + \frac{1}{2m}\left(\frac{\partial S}{\partial q}\right)^2 + \frac{1}{2}kq^2 = 0 \tag{3.310}$$

It turns out in this case that a solution exists of the form

$$S = -\omega t + S_0 \tag{3.311}$$

where S_0 is independent of t, and ω is independent of q. This may be seen as a type of separation of variables. Substituting into the Hamilton-Jacobi equation,

$$-\omega + \frac{1}{2m}\left(\frac{\partial S_0}{\partial q}\right)^2 + \frac{1}{2}kq^2 = 0 \tag{3.312}$$

or

$$\frac{\partial S_0}{\partial q} = \sqrt{m\left(\omega - kq^2\right)} \tag{3.313}$$

This has solution

$$S_0\left(q\right) = \int \sqrt{m\left(\omega - kq^2\right)}\, dq = \sqrt{\frac{m\omega^2}{k}}\left(\frac{1}{2}x\sqrt{1-x^2} + \frac{1}{2}\sin^{-1} x\right) \tag{3.314}$$

where $x^2 = kq^2/\omega$. The transformation equations are

$$p = \frac{\partial S}{\partial q} = \sqrt{m\left(\omega - kq^2\right)} \tag{3.315}$$

and $Q = \partial S/\partial P$. In order to determine Q, we need to decide what is P, which is supposed to be a "constant of integration" associated with solving the Hamilton-Jacobi equation, depending on the initial conditions. In this example, the separation constant ω will serve. For example, if at $t = 0$, the oscillator is at rest $p = 0$ and $q = q_0$, then by (3.315), the value of ω is kq_0^2. Identifying $P = \omega$, we see that from

$$S = -\omega t + S_0\left(q, \omega\right), \tag{3.316}$$

we have that

$$Q = \frac{\partial S}{\partial P} = \frac{\partial S}{\partial \omega} = -t + \frac{\partial S_0}{\partial \omega} = -t + \frac{\partial}{\partial \omega}\int \sqrt{m\left(\omega - kq^2\right)}\, dq \tag{3.317}$$

$$= -t + \sqrt{m}\int \frac{1}{\sqrt{\omega - kq^2}}\, dq \tag{3.318}$$

$$= -t + \sqrt{\frac{m}{k}}\sin^{-1}\left(q\sqrt{\frac{k}{\omega}}\right) \tag{3.319}$$

In the new coordinate system in phase space, $H' = 0$ and so Q is a constant of the motion determined by the initial conditions. If we write $Q = Q_0$ for all time, the transformation may be inverted to yield

$$q = \sqrt{\frac{\omega}{k}}\sin\left[\sqrt{\frac{k}{m}}\left(t + Q_0\right)\right] = \sqrt{\frac{P_0}{k}}\sin\left[\sqrt{\frac{k}{m}}\left(t + Q_0\right)\right] \tag{3.320}$$

where $P_0 = \omega$ is the constant value of the new momentum coordinate. As expected, the motion of the oscillator is sinusoidal, with the initial conditions determining the amplitude and phase of the oscillation. Note that in this case, we actually carried out the integration in (3.314) to get an explicit form for $S_0\left(q\right)$, but this is in fact not used, since only the derivatives of S appear in the transformation equations.

Example: Motion under gravity

As a second example of finding a transformation that reduces the Hamiltonian to zero, consider the projectile with Hamiltonian

$$H\left(q, p, t\right) = \frac{p_1^2 + p_2^2}{2m} + mgq_2. \tag{3.321}$$

The Hamilton-Jacobi equation for the canonical transformation is

$$\frac{\partial G}{\partial t} + H\left(q_1, q_2, \frac{\partial G}{\partial q_1}, \frac{\partial G}{\partial q_2}, t\right) = 0 \tag{3.322}$$

or

$$\frac{\partial G}{\partial t}+\frac{1}{2m}\left[\left(\frac{\partial G}{\partial q_1}\right)^2+\left(\frac{\partial G}{\partial q_2}\right)^2\right]+mgq_2=0. \tag{3.323}$$

We solve this by trying a separable solution of the form

$$G\left(q_1,q_2,t\right)=G_1\left(q_1\right)+G_2\left(q_2\right)+T\left(t\right) \tag{3.324}$$

which we substitute into the Hamilton-Jacobi equation, yielding

$$T'\left(t\right)+\frac{1}{2m}\left(G_1'\right)^2+\left\{\frac{1}{2m}\left(G_2'\right)^2+mgq_2\right\}=0. \tag{3.325}$$

We see that T' is a function of t alone, $G_1'^2/\left(2m\right)$ is a function of q_1 alone and the term in braces is a function of q_2 alone. Since they sum to zero, each must be equal to a constant. We may set

$$\begin{aligned}\frac{\left(G_1'\right)^2}{2m} &= P_1 &(3.326)\\ \frac{1}{2m}\left(G_2'\right)^2+mgq_2 &= P_2 &(3.327)\\ T' &= -\left(P_1+P_2\right) &(3.328)\end{aligned}$$

where we have defined two of the separation constants to be the new momenta. These equations may be integrated to yield

$$\begin{aligned}T\left(t\right) &= -\left(P_1+P_2\right)t &(3.329)\\ G_1\left(q_1\right) &= \sqrt{2mP_1}\,q_1 &(3.330)\\ G_2\left(q_2\right) &= \int\sqrt{2m\left(P_2-mgq_2\right)}\,\mathrm{d}q_2 &(3.331)\end{aligned}$$

so that

$$G\left(q,P,t\right)=\sqrt{2mP_1}\,q_1+\int\sqrt{2m\left(P_2-mgq_2\right)}\,\mathrm{d}q_2-\left(P_1+P_2\right)t \tag{3.332}$$

Note that G is defined up to an unimportant additive constant.

The function G now contains all the information needed to solve the problem within its partial derivatives. In particular we can find q_i and p_i in terms of the constants of the motion Q_i and P_i. From the equations of canonical transformation, we know that

$$Q_i=\frac{\partial G}{\partial P_i},\quad p_i=\frac{\partial G}{\partial q_i}\quad\text{and}\quad H'=0=H+\frac{\partial G}{\partial t} \tag{3.333}$$

so that, for example,

$$p_1=\frac{\partial G}{\partial q_1}=\sqrt{2mP_1} \tag{3.334}$$

Thus $P_1=p_1^2/\left(2m\right)$ is a constant of the motion.

Also, since $H'=0$, all the Q_i are constants of the motion as well. Thus

$$Q_1=\frac{\partial G}{\partial P_1}=\sqrt{\frac{m}{2P_1}}\,q_1-t \tag{3.335}$$

is constant, and so

$$q_1=\sqrt{\frac{2P_1}{m}}\left(t+Q_1\right). \tag{3.336}$$

Since $P_1=\frac{1}{2}mv_x^2$, this gives $q_1=v_x\left(t+Q_1\right)$, as expected for a projectile.

Similarly, we find that

$$p_2=\frac{\partial G}{\partial q_2}=\sqrt{2m\left(P_2-mgq_2\right)} \tag{3.337}$$

so that

$$P_2 = \frac{p_2^2}{2m} + mgq_2 \tag{3.338}$$

is also a constant of the motion. We also have

$$\begin{aligned} Q_2 &= \frac{\partial G}{\partial P_2} = \int \frac{1}{\sqrt{2m\left(P_2 - mgq_2\right)}}\,\mathrm{d}q_2 - t \\ &= -\frac{1}{mg}\sqrt{2m\left(P_2 - mgq_2\right)} - t \end{aligned} \tag{3.339}$$

Hence

$$q_2 = \left[\frac{P_2 - \frac{1}{2}m\left(gQ_2\right)^2}{mg}\right] - gQ_2 t - \frac{1}{2}gt^2 \tag{3.340}$$

again as expected for the projectile.

3.14.2 Relationship with Quantum Mechanics

For the projectile, consider a plot of the contours of $G\left(q_1, q_2, P_1, P_2, t\right)$ as a function of q_1 and q_2 for fixed values of P_1 and P_2, where

$$G\left(q_1, q_2, P_1, P_2, t\right) = \sqrt{2mP_1}\,q_1 - \frac{2m}{3}\sqrt{2g}\left(\frac{P_2}{mg} - q_2\right)^{3/2} - \underbrace{(P_1 + P_2)t}_{E} \tag{3.341}$$

If we plot the path of the particle on these contours, it is found that the trajectory cuts the level curves of G at right angles.This geometrical relationship between the trajectory and the function G follows from

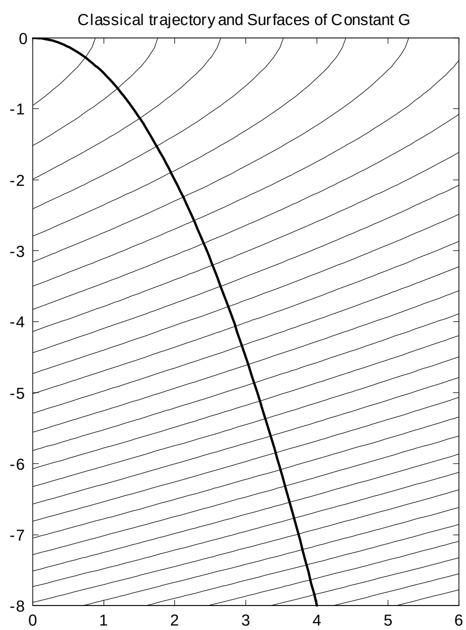

Figure 3.3 Contours of the generating function $G\left(q_1, q_2, P_1, P_2, t\right)$ of the canonical transformation which makes $H' = 0$ for a projectile, together with the classical trajectory $\left(q_1\left(t\right), q_2\left(t\right)\right)$ for constant P_1, and P_2.

the equation $p_i = \partial G/\partial q_i$ or $\mathbf{p} = \boldsymbol{\nabla} G$. Since the momentum is the gradient of G, it is perpendicular to the level surfaces of G, and is large when the level surfaces are close together. This resembles the relationship between rays and wavefronts, and if we treat the level surfaces of G as being wavefronts, the wavelength is *inversely proportional* to p.

From the dependence of G on time, we see that the level surfaces shown move as t increases. The rate at which wavefronts pass a point (i.e., the "frequency" of the wave) is proportional to $P_1 + P_2$, or the energy.

In quantum mechanics, we have a de Broglie wave for which $\lambda = h/p$ and $\nu = E/h$. The quantity analogous to the action G is the *phase* of the wave function.

Indeed, if we consider the time-dependent Schrödinger equation

$$\mathrm{i}\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial q^2} + V\psi \tag{3.342}$$

and write the wave function as

$$\psi(q,t) \propto \exp\left[\frac{\mathrm{i}}{\hbar}\Phi(q,t)\right] \tag{3.343}$$

where Φ is $\hbar$ times the phase of the de Broglie wave, then substituting this solution into the Schrödinger equation yields

$$\frac{\partial\Phi}{\partial t} + \frac{1}{2m}\left[\left(\frac{\partial\Phi}{\partial q}\right)^2 - i\hbar\left(\frac{\partial^2\Phi}{\partial q^2}\right)\right] + V(q) = 0. \tag{3.344}$$

In the limit of $\hbar \to 0$, we find that

$$\frac{\partial\Phi}{\partial t} + \frac{1}{2m}\left(\frac{\partial\Phi}{\partial q}\right)^2 + V(q) = 0 \tag{3.345}$$

which coincides with the Hamilton-Jacobi equation. From this viewpoint, classical mechanics is the "ray optics of wave mechanics".

3.14.3 Time-independent Hamiltonians

We now consider the case of a time-independent Hamiltonian $H(q,p)$ and show that there is now a time-independent generating function $G(q,P)$ such that all the new "position" coordinates Q_i are cyclic. When the Hamiltonian is time-independent, it is a constant of the motion (depending on the initial conditions) which we may write as E. Often, this will just be the energy (e.g., if the relationship between the generalized coordinates and the inertial coordinates are time-independent), but in any case it will not change with time. In the new phase-space coordinate system, we may identify H_0 as one of the constant momentum coordinates, say P_1.

In the time-dependent Hamilton-Jacobi equations (3.308), if H is in fact independent of time, we find that

$$\frac{\partial S}{\partial t} + H\left(q_1, ..., q_s, \frac{\partial S}{\partial q_1}, ..., \frac{\partial S}{\partial q_s}\right) = 0. \tag{3.346}$$

Since H is a constant of the motion and is equal to $E = P_1$ for all time, we see that the dependence of S on t is simple,

$$\frac{\partial S}{\partial t} + P_1 = 0 \tag{3.347}$$

so that

$$S(q,P,t) = W(q,P) - P_1 t \tag{3.348}$$

where $W(q,P)$ is called Hamilton's characteristic function or the time-independent action. Substituting this back into the Hamilton-Jacobi equation, we find that

$$H\left(q_1, ..., q_s, \frac{\partial W}{\partial q_1}, ..., \frac{\partial W}{\partial q_s}\right) = P_1 \tag{3.349}$$

which is known as the time-independent Hamilton-Jacobi equation. The solution of this partial differential equation $W(q,P)$ gives the desired time-independent generating function $G(q,P)$. As before, there are s constants of integration, one of which is a trivial additive constant. The remaining $s-1$ constants may be identified with the remaining conjugate momenta P_2 through P_s.

In the new coordinate system (Q,P), the Hamiltonian H' is given by (3.298) as

$$H'(Q,P) = H(q,p) \tag{3.350}$$

since the generating function W is independent of time, and so $\partial W/\partial t = 0$. Since we have chosen P_1 to be the constant value of the Hamiltonian,

$$H'(Q,P) = P_1 \tag{3.351}$$

so that not only are all the Q_i cyclic, but so are $P_2, ..., P_s$. The canonical equations are easily seen to be

$$\dot{P}_i = 0 \text{ for } i = 1, ..., s \tag{3.352}$$

and

$$\dot{Q}_i = \frac{\partial H'}{\partial P_i} = \begin{cases} 1 & \text{for } i = 1 \\ 0 & \text{otherwise} \end{cases} \tag{3.353}$$

These may be integrated directly to yield

$$\begin{aligned} P_1(t) &= E \text{ and } P_i(t) = \alpha_i \text{ for } i = 2, ..., s, & (3.354) \\ Q_1(t) &= t + \beta_1 \text{and } Q_i(t) = \beta_i \text{ for } i = 2, ..., s & (3.355) \end{aligned}$$

where α and β are constants depending on the initial conditions.

Example: The Central Force Problem

For the central force problem in plane polar coordinates,

$$L = \frac{1}{2}m\left(\dot{\rho}^2 + \rho^2\dot{\phi}^2\right) + \frac{k}{\rho} \tag{3.356}$$

so that

$$p_r = m\dot{\rho} \text{ and } p_\phi = m\rho^2\dot{\phi} \tag{3.357}$$

and

$$H = \frac{p_r^2}{2m} + \frac{p_\phi^2}{2m\rho^2} - \frac{k}{\rho} \tag{3.358}$$

The Hamilton-Jacobi equations are

$$\frac{1}{2m}\left(\frac{\partial W}{\partial \rho}\right)^2 + \frac{1}{2m\rho^2}\left(\frac{\partial W}{\partial \phi}\right)^2 - \frac{k}{\rho} = E \tag{3.359}$$

We try a separable solution of the form

$$W(\rho,\phi) = W_\rho(\rho) + W_\phi(\phi) \tag{3.360}$$

which when substituted into the Hamilton-Jacobi equations gives

$$\frac{1}{2m}\left(\frac{\partial W_\rho}{\partial \rho}\right)^2 + \frac{1}{2m\rho^2}\left(\frac{\partial W_\phi}{\partial \phi}\right)^2 - \frac{k}{\rho} = E \tag{3.361}$$

Since we can write

$$\left(\frac{\partial W_\phi}{\partial \phi}\right)^2 = 2m\rho^2\left\{E + \frac{k}{\rho} - \frac{1}{2m}\left(\frac{\partial W_\rho}{\partial \rho}\right)^2\right\} \tag{3.362}$$

where the left hand side is a function of ϕ alone and the right hand side is a function of ρ alone, both sides must in fact be equal to a constant, which we may denote as P_2^2 (Recall that $P_1 = E$). Thus

$$\frac{\partial W_\phi}{\partial \phi} = P_2 \text{ or } W_\phi = P_2\phi \tag{3.363}$$

and

$$2m\rho^2\left\{E + \frac{k}{\rho} - \frac{1}{2m}\left(\frac{\partial W_\rho}{\partial \rho}\right)^2\right\} = P_2^2 \tag{3.364}$$

so that

$$W_\rho = \int\sqrt{2m\left(E + \frac{k}{\rho} - \frac{P_2^2}{2m\rho^2}\right)}\,d\rho \tag{3.365}$$

It is easy to find a physical significance for the constant of the motion P_2. Since by (3.296),

$$P_2 = \frac{\partial W_\phi}{\partial \phi} = \frac{\partial W}{\partial \phi} = p_\phi \tag{3.366}$$

we see that P_2 is just the angular momentum, which we previously denoted by l.

We may use the transformation equations (3.297) to obtain the path in configuration space $q(t)$ taken by the particle. These are

$$Q_i = \frac{\partial W}{\partial P_i} = \frac{\partial W_\rho}{\partial P_i} + \frac{\partial W_\phi}{\partial P_i} \tag{3.367}$$

For $i = 1$, we know that the solution is $Q_1 = t + \beta_1$, while for all other values of i, $Q_i = \beta_i$ is a constant of the motion. The equation for $i = 1$ gives the way in which the radius ρ depends on time as an explicit quadrature (integral):

$$t + \beta_1 = Q_1 = \frac{\partial}{\partial E} \int \sqrt{2m\left(E + \frac{k}{\rho} - \frac{P_2^2}{2m\rho^2}\right)}\, d\rho = \int \frac{m}{\sqrt{2m\left(E + \frac{k}{\rho} - \frac{P_2^2}{2m\rho^2}\right)}} d\rho \tag{3.368}$$

Of greater interest is the second equation which is independent of time, since Q_2 is a constant of the motion. This relates the variables ρ and ϕ directly, without involving t. i.e., it gives the equation of the orbit directly.

$$Q_2 = \frac{\partial}{\partial P_2} \int \sqrt{2m\left(E + \frac{k}{\rho} - \frac{P_2^2}{2m\rho^2}\right)}\, d\rho + \frac{\partial}{\partial P_2}(P_2\phi) \tag{3.369}$$

$$= -\int \frac{P_2}{\rho\sqrt{(2Em\rho^2 + 2km\rho - P_2^2)}}\, d\rho + \phi \tag{3.370}$$

Putting $u = 1/\rho$ simplifies the calculation of the integral:

$$Q_2 = \int \left(\frac{2mE}{P_2^2} + \left(\frac{mk}{P_2^2}\right)^2 - \left(u - \frac{mk}{P_2^2}\right)^2\right)^{-1/2} du + \phi \tag{3.371}$$

Since Q_2 is a constant of motion, we can set it equal to ϕ_0 (rather than β_2) and perform the integration to give

$$\phi - \phi_0 = \cos^{-1} \frac{u - \frac{mk}{P_2^2}}{\sqrt{\frac{2mE}{P_2^2} + \left(\frac{mk}{P_2^2}\right)^2}} \tag{3.372}$$

or

$$u = \frac{1}{\rho} = \frac{mk}{P_2^2}\left\{1 + \sqrt{1 + \frac{2P_2^2 E}{mk^2}} \cos(\phi - \phi_0)\right\} \tag{3.373}$$

Identifying $P_2 = l$, the angular momentum, we see that this is a conic section with semi-latus rectum $l^2/(mk)$ and eccentricity

$$e = \sqrt{1 + \frac{2l^2 E}{mk^2}} \tag{3.374}$$

exactly as we determined in chapter 1. Just as we can make a connection between the time-dependent Hamilton-Jacobi equation and the time-dependent Schrödinger equation, it is also possible to relate the time-independent forms of these equations.