Classical Mechanics

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Hilary Term 1999

Books

T.W.B. Kibble, *Classical Mechanics*, Longman Scientific (about £18): overall the most suitable book.

L.D. Landau & E. Lifshitz, *Classical Mechanics*, IoP Publishing: one of the best books in the classic series on theoretical physics.

Tai L. Chow, *Classical Mechanics*, Wiley, (about £23): a useful source of additional information but marred by too many typos.

V.I. Arnold, *Mathematical Methods of Mechanics*, Springer: a uniquely insightful book but too sophisticated for most undergraduates.

1 Lagrangian Mechanics

Mechanics as formulated by Newton suffers from two important limitations: (i) it deals with particles; (ii) it describes their motion in special Cartesian coordinate systems: if the numbers x_i are the coordinates of a particle in an inertial Cartesian coordinate system, then the position of the particle when subjected for a force with components $f_i(t)$ may be determined by solving the differential equations $\ddot{x}_i = f_i(t)$. Since an extended body can be decomposed into its consituent particles, and its motion, once determined, can be transformed into any reference frame, Newton's machinery enables us to determine the motion of any body in any reference frame notwithstanding these limitations. But in practice it is better to determine the dynamics of complex dynamical systems from a more powerful principle than Newton's laws of motion. Lagrangian dynamics provides just such a principle.

Let q_i $i = 1, \ldots, N$ be **generalized coordinates** for some system. That is, these N numbers enable us to specify precisely the system's configuration. For example, six numbers suffice to specify a configuration of a rigid body such as a hard-boiled egg: we can take (q_1, q_2, q_3) to be the coordinates in some system, such as spherical polar coordinates, of the body's centre of mass, and (q_4, q_5, q_6) to be the three angles that are required to define its orientation. (Box 1 defines **Euler angles**, the standard angles for specifying the orientation of a rigid body.) The number of generalized coordinates N required by a system is called the system's **number of degrees of freedom**.

At each instant our system is at some point in **configuration space** – an imaginary N-dimensional space for which the q_i constitute Cartesian coordinates. As the system moves, its representative point in configuration space sweeps out a path $\mathbf{q}(t)$. Since Newton's laws of motion are 2nd order in time, we expect this path to be uniquely determined by specifying at some time t_1 both $\mathbf{q}(t_1)$ and $\dot{\mathbf{q}}(t_1)$. In Lagrangian mechanics we take rather a different point of view: we do not specify $\dot{\mathbf{q}}(t_1)$ but instead specify $\mathbf{q}$ at a second time t_2. That is, we ask what path does our system follow if its configuration at time t_1 is $\mathbf{q}(t_1)$ and at time t_2 is $\mathbf{q}(t_2)$? For reasons that give deep insight into the connection between classical and quantum mechanics, it turns out that the sought-after path $\mathbf{q}(t)$ is the path that extremizes a certain quantity S. Our next task is to introduce the mathematical machinery required to define S and to show that it is extremized on the Newtonian path. At the end of the course we shall investigate the connection between the extremization of S and quantum mechanics.

1.1 Paths, functionals & the calculus of variations

Before a 'plane takes off from New York for London, its computer chooses an optimal path $\mathbf{x}(t)$; i.e., it finds that sequence of longitudes, latitudes and altitudes at each moment t of the flight which, given prevailing winds, will get it to London at the prescribed time with least expenditure of fuel. The quantity of fuel required to get to London in a given time is a single number F that depends on the whole path $\mathbf{x}(t)$; one says that F is a **functional** $F[\mathbf{x}]$ of the path $\mathbf{x}(t)$.

The simplest functionals are integrals along the path of functions of $\mathbf{x}(t)$ and its derivatives with respect to t:

$$\begin{aligned} F_1[\mathbf{x}] &\equiv \int_{t_1}^{t_2} |\mathbf{x}(t)|^2 \, \mathrm{d}t \\ F_2[\mathbf{x}] &\equiv \int_{t_1}^{t_2} |\dot{\mathbf{x}}(t)|^2 \, \mathrm{d}t \\ F_3[\mathbf{x}] &\equiv \int_{t_1}^{t_2} \mathbf{x} \cdot \dot{\mathbf{x}}(t) \, \mathrm{d}t \\ &\cdots\cdots \end{aligned}$$

How do we find the path that minimizes a functional

$$F[\mathbf{x}] \equiv \int_{t_1}^{t_2} f(\mathbf{x}, \dot{\mathbf{x}}, t) \, \mathrm{d}t \ ? \tag{1.1}$$

Let $\overline{\mathbf{x}}(t)$ be the minimizing path and let $\boldsymbol{\eta}(t)$ be a small variation, so that $\mathbf{x}(t) \equiv \overline{\mathbf{x}}(t) + \boldsymbol{\eta}(t) \approx \overline{\mathbf{x}}(t)$. We insist on $\boldsymbol{\eta}$ vanishing at $t = t_1, t_2$ so that $\overline{\mathbf{x}}(t)$ and the modified path both start and finish at the same places at the same times. Then[1]

$$\begin{aligned} F[\overline{\mathbf{x}}] \le F[\mathbf{x}] &= \int_{t_1}^{t_2} f(\overline{\mathbf{x}} + \boldsymbol{\eta}, \dot{\overline{\mathbf{x}}} + \dot{\boldsymbol{\eta}}, t) \, \mathrm{d}t \\ &= \int_{t_1}^{t_2} \Big(f(\overline{\mathbf{x}}, \dot{\overline{\mathbf{x}}}, t) + \frac{\partial f}{\partial \mathbf{x}} \cdot \boldsymbol{\eta} + \frac{\partial f}{\partial \dot{\mathbf{x}}} \cdot \dot{\boldsymbol{\eta}} + \cdots \Big) \, \mathrm{d}t \\ &= F[\overline{\mathbf{x}}] + \int_{t_1}^{t_2} \Big(\frac{\partial f}{\partial \mathbf{x}} \cdot \boldsymbol{\eta} + \frac{\partial f}{\partial \dot{\mathbf{x}}} \cdot \dot{\boldsymbol{\eta}} + \cdots \Big) \, \mathrm{d}t. \end{aligned} \tag{1.2}$$

We now integrate by parts the second term in the integral of the last line:

$$\int_{t_1}^{t_2} \frac{\partial f}{\partial \dot{\mathbf{x}}} \cdot \dot{\boldsymbol{\eta}} \, \mathrm{d}t = \Big[\frac{\partial f}{\partial \dot{\mathbf{x}}} \cdot \boldsymbol{\eta} \Big]_{t_1}^{t_2} - \int_{t_1}^{t_2} \frac{\mathrm{d}}{\mathrm{d}t} \Big(\frac{\partial f}{\partial \dot{\mathbf{x}}} \Big) \cdot \boldsymbol{\eta} \, \mathrm{d}t. \tag{1.3}$$

Since $\boldsymbol{\eta}(t_1) = \boldsymbol{\eta}(t_2) = 0$, the [.] vanishes. Putting this into (1.2) we have

$$0 \ge F[\mathbf{x}] - F[\overline{\mathbf{x}}] = \int_{t_1}^{t_2} \Big[\Big(\frac{\partial f}{\partial \mathbf{x}} - \frac{\mathrm{d}}{\mathrm{d}t} \frac{\partial f}{\partial \dot{\mathbf{x}}} \Big) \cdot \boldsymbol{\eta} + \cdots \Big] \, \mathrm{d}t. \tag{1.4}$$

This relation must hold for any $\boldsymbol{\eta}$, no matter how small. So the higher terms indicated by $+\cdots$ can be neglected. The remaining integrand is proportional to $\boldsymbol{\eta}$, so if it were non-zero for some particular function $\boldsymbol{\eta}(t)$, it would have the opposite sign for $\boldsymbol{\eta}' \equiv -\boldsymbol{\eta}$. The inequality on the extreme left would then be violated for one of $\boldsymbol{\eta}$ of $\boldsymbol{\eta}'$. Hence

[1] We use the convention that $\mathbf{y} \cdot \dfrac{\partial}{\partial \mathbf{x}} \equiv \displaystyle\sum_i y_i \cdot \frac{\partial}{\partial x_i}$.

the integral must vanish for all $\boldsymbol{\eta}$. This is possible only if the coefficient of $\boldsymbol{\eta}$ vanishes *for all* $t_1 < t < t_2$: if it did not vanish for some t, say t', the integral would fail to vanish for the particular choice $\boldsymbol{\eta} = \delta(t - t')$. So $\overline{\mathbf{x}}(t)$ minimizes F if and only if

$$\frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial f}{\partial \dot{\mathbf{x}}} - \frac{\partial f}{\partial \mathbf{x}} = 0 \tag{1.5}$$

all along the path $\overline{x}(t)$.

Eq (1.5) is called the **Euler-Lagrange equation** ('EL eqn'), and the theory that underlies it is called **the calculus of variations**. It is one of the few results we have in the theory of functionals—one everywhere in physics encounters problems that cry out for a fully fledged calculus of functions that shows how to integrate, Taylor expand, exponentiate etc functionals the way we do functions.

Legend has it that the calculus of variations was invented by Newton after dinner one evening to solve this challenge problem (set in 1695 by Johann Bernoulli):

Example 1

A bead slides on a smooth wire that passes through two rings, one at the origin, the other at $(x', y', z') = (x_0, 0, -z_0)$ with $z_0 > 0$. To what curve (the 'brachystochrone') must the wire be bent in order to minimize the time required for the bead to slide from rest at the upper ring to the lower ring?

Solution: The optimal curve obviously lies in the plane $y' = 0$. It is convenient to work in coordinates (x, y, z) such that z increases downwards. Then the time of flight is

$$\tau = \int_0^{z_0} \frac{\mathrm{d}z}{\dot{z}}.$$

But $\frac{1}{2}(\dot{x}^2 + \dot{z}^2) = gz$, so $\dot{z} = \sqrt{2gz/[(\mathrm{d}x/\mathrm{d}z)^2 + 1]}$ and

$$\tau = \int_0^{z_0} \frac{\mathrm{d}z}{\sqrt{2gz}} \sqrt{\left(\frac{\mathrm{d}x}{\mathrm{d}z}\right)^2 + 1}. \tag{1.6}$$

We need to minimize $\tau[x(z)]$ from (1.6) with respect to the path $x(z)$. We may use the EL-eqn (1.5) provided we make the substitutions

$$t \to z, \qquad f\left(x, \frac{\mathrm{d}x}{\mathrm{d}z}, z\right) = \frac{1}{\sqrt{2gz}} \sqrt{\left(\frac{\mathrm{d}x}{\mathrm{d}z}\right)^2 + 1}. \tag{1.7}$$

Since f does not depend on x, the optimal path satisfies

$$0 = \frac{\mathrm{d}}{\mathrm{d}z}\left(\frac{\mathrm{d}x/\mathrm{d}z}{\sqrt{z}\sqrt{(\mathrm{d}x/\mathrm{d}z)^2 + 1}}\right),$$

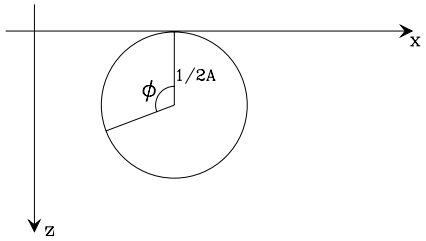
which implies

$$x(z) = \int_0^z \sqrt{\frac{Az}{1 - Az}}\, \mathrm{d}z,$$

where A is a constant of integration. In terms of variable $\sin^2\theta \equiv Az$ the answer is

$$x = \frac{1}{A}\left(\theta - \tfrac{1}{2}\sin 2\theta\right). \tag{1.8}$$

If we write $\phi \equiv 2\theta$ this may be written $z = (1-\cos\phi)/2A$, $x = (\phi - \sin\phi)/2A$, which is a cycloid with the origin at its cusp. A may be determined by first solving $x_0/z_0 = (\phi_0 - \sin\phi_0)/(1-\cos\phi_0)$ for ϕ_0 and then using this value in $A = \frac{1}{2}(1-\cos\phi_0)/z_0$.



1.2 The Principle of Least Action

As was stated above, the path $\mathbf{q}(t)$ taken through configuration space by a dynamical system can be found by identifying the path which extremizes a quantity $S[\mathbf{q}(t)]$ between specified locations $\mathbf{q}(t_1)$ and $\mathbf{q}(t_2)$ of the system at given times t_1, t_2. S is called the **action** and is usually (but not invariably) minimized by the dynamical path. Hence the idea that the dynamical path can be determined by extremizing S is called the **principle of least action**.

S takes the form of an integral over t of a function L of $\mathbf{q}$ and $\dot{\mathbf{q}}$:

$$S = \int_{t_1}^{t_2} L(\mathbf{q}, \dot{\mathbf{q}})\,\mathrm{d}t. \tag{1.9}$$

Here L is just a function (rather than a functional) of its arguments. It is called the **Lagrangian** of the system. Since the dynamical evolution of the system is entirely determined by L, writing down L amounts to specifying the physical content of the system.

There is no entirely general rule for writing down L – one would hardly expect one rule to be valid for every possible dynamical system – but there is a rule that works for most simple systems: L is the *difference* between the system's kinetic energy T and its potential energy V;

$$L = T - V. \tag{1.10}$$

Let's se how this works out in a simple case: a particle of mass m moving in a gravitaional potential $\Phi(\mathbf{x})$. Now $T = \frac{1}{2}m\dot{\mathbf{x}}^2$, $V = m\Phi$. So $L(\mathbf{x}, \dot{\mathbf{x}}) = \frac{1}{2}m\dot{\mathbf{x}}^2 - m\Phi(\mathbf{x})$. Setting $f = L$ in the EL equations (1.5) we obtain the equations of motion as

$$\frac{\mathrm{d}}{\mathrm{d}t}m\dot{\mathbf{x}} + m\frac{\partial\Phi}{\partial\mathbf{x}} = 0 \tag{1.11}$$

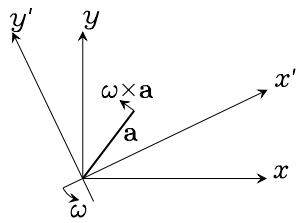
as required.

Exercise (1):

Consider a shell that is fired at t_1 and hits its target at t_2. Explain in general terms why its action would be larger if it flew on either a higher or a lower trajectory than it actually does.

1.3 Equations of motion from Lagrangians

The Lagrangian provides a neat way of calculating the eqns of motion of a particle when referred to an odd coordinate system because it is easier to transform a single function to new-fangled coordinates that a set of eqns of motion. Consider, for example, motion in a rotating frame.



Suppose both primed and unprimed coordinates share the same origin, but the primed coordinates rotate with angular velocity $\boldsymbol{\omega}$ with respect to the unprimed coordinates, which are inertial. Then

$$\mathbf{v}_{\text{inertial}} = \dot{\mathbf{r}}' + \boldsymbol{\omega} \times \mathbf{r}'.$$

So written in terms of the primed coordinates the k.e. is

$$\begin{aligned} T &= \tfrac{1}{2}mv^2 = \tfrac{1}{2}m\left|\dot{\mathbf{r}}' + \boldsymbol{\omega} \times \mathbf{r}'\right|^2 \\ &= \tfrac{1}{2}m|\dot{\mathbf{r}}'|^2 + m\dot{\mathbf{r}}' \cdot (\boldsymbol{\omega} \times \mathbf{r}') + \tfrac{1}{2}m|\boldsymbol{\omega} \times \mathbf{r}'|^2 \end{aligned} \tag{1.12}$$

The p.e. is just $V(\mathbf{r}', t)$ so

$$L = \tfrac{1}{2}m|\dot{\mathbf{r}}'|^2 + m\dot{\mathbf{r}}' \cdot (\boldsymbol{\omega} \times \mathbf{r}') + \tfrac{1}{2}m|\boldsymbol{\omega} \times \mathbf{r}'|^2 - V. \tag{1.13}$$

In writing down the EL-eqns we recall that $\dot{\mathbf{r}}' \cdot (\boldsymbol{\omega} \times \mathbf{r}') = \mathbf{r}' \cdot (\dot{\mathbf{r}}' \times \boldsymbol{\omega})$. We then find

$$\begin{aligned} 0 &= \frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial L}{\partial \dot{\mathbf{r}}'} - \frac{\partial L}{\partial \mathbf{r}'} \\ &= \frac{\mathrm{d}}{\mathrm{d}t}(m\dot{\mathbf{r}}' + m\boldsymbol{\omega} \times \mathbf{r}') - \left[m\dot{\mathbf{r}}' \times \boldsymbol{\omega} + \frac{\partial}{\partial \mathbf{r}'}\Big(\tfrac{1}{2}m|\boldsymbol{\omega} \times \mathbf{r}'|^2 - V\Big)\right]. \end{aligned} \tag{1.14}$$

Collecting everything together we have finally

$$m\ddot{\mathbf{r}}' = 2m\dot{\mathbf{r}}' \times \boldsymbol{\omega} - \frac{\partial V_{\text{eff}}}{\partial \mathbf{r}'} \quad \text{where} \quad V_{\text{eff}} \equiv V - \tfrac{1}{2}m|\boldsymbol{\omega} \times \mathbf{r}'|^2. \tag{1.15}$$

In a rotating frame there is a contribution to the "acceleration" $\ddot{\mathbf{r}}'$ from the **Coriolis force** $2m\boldsymbol{\omega} \times \dot{\mathbf{r}}'$, and the potential needs to be augmented by a term that gives rise to the **centrifugal force** $\mathbf{r}\omega^2 - (\boldsymbol{\omega} \cdot \mathbf{r}')\boldsymbol{\omega}$. Forces such as these, which appear because one's frame is non-inertial, are called **pseudo-forces**.

A second example illustrates that Lagrangians work even for coordinates that depend explicitly on time. In cosmology it is handy to use 'comoving' coordinates such that the spatial coordinates of particles that move apart as the Universe expands are

constant. Let the primed system be inertial and the unprimed system comoving. Then $\mathbf{r}' = a(t)\mathbf{r}$, where $a(t)$ is the cosmic scale factor. So

$$T = \tfrac{1}{2}m\dot{\mathbf{r}}'^2 = \tfrac{1}{2}m(a\dot{\mathbf{r}} + \dot{a}\mathbf{r})^2. \tag{1.16}$$

Writing the potential energy as $V = m\Phi$ the EL eqns are

$$0 = \frac{\mathrm{d}}{\mathrm{d}t}\big[m(a\dot{\mathbf{r}} + \dot{a}\mathbf{r})a\big] - m(a\dot{\mathbf{r}} + \dot{a}\mathbf{r})\dot{a} + m\frac{\partial\Phi}{\partial\mathbf{r}}.$$

Cleaning up we get

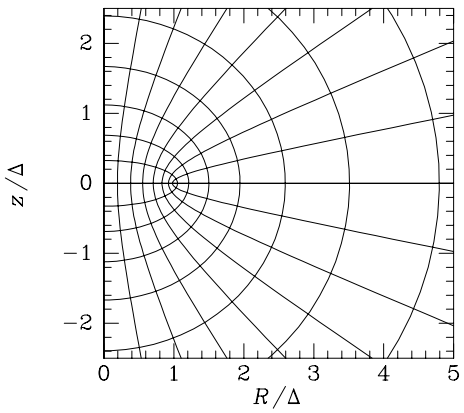
$$\ddot{\mathbf{r}} + 2\frac{\dot{a}}{a}\dot{\mathbf{r}} + \frac{\ddot{a}}{a}\mathbf{r} = -\frac{1}{a^2}\frac{\partial\Phi}{\partial\mathbf{r}}. \tag{1.17}$$

A final example illustrates how to get T in a weird curvilinear coordinate system. Oblate spheroidal coordinates (u, v, ϕ) are related to regular cylindrical polars (R, z, ϕ) by

$$R = \Delta\cosh u\cos v \quad ; \quad z = \Delta\sinh u\sin v. \tag{1.18}$$

Slightly changing u, v and ϕ in turn while leaving the other coordinates alone, generates small displacements

$$\boldsymbol{\delta}_u = \Delta\delta u(\sinh u\cos v\hat{\mathbf{R}} + \cosh u\sin v\hat{\mathbf{z}})$$
$$\boldsymbol{\delta}_v = \Delta\delta v(-\cosh u\sin v\hat{\mathbf{R}} + \sinh u\cos v\hat{\mathbf{z}})$$
$$\boldsymbol{\delta}_\phi = R\delta\phi\hat{\boldsymbol{\phi}}.$$



It is easy to check that these three displacement vectors are mutually perpendicular. So the distance one goes on changing all of (u, v, ϕ) simultaneously is

$$\begin{aligned}\mathrm{d}s^2 &= |\boldsymbol{\delta}_u + \boldsymbol{\delta}_v + \boldsymbol{\delta}_\phi|^2 = \delta_u^2 + \delta_v^2 + \delta_\phi^2 \\ &= \Delta^2\big[(\delta u)^2(\sinh^2 u\cos^2 v + \cosh^2 u\sin^2 v) \\ &\qquad + (\delta v)^2(\cosh^2 u\sin^2 v + \sinh^2 u\cos^2 v) + (\delta\phi)^2\cosh^2 u\cos^2 v\big] \\ &= \Delta^2\big\{(\cosh^2 u - \cos^2 v)[(\delta u)^2 + (\delta v)^2] + \cosh^2 u\cos^2 v(\delta\phi)^2\big\}.\end{aligned} \tag{1.19}$$

Dividing through by $\mathrm{d}t^2$ we get the kinetic energy in terms of $(\dot{u}, \dot{v}, \dot{\phi})$:

$$T = \tfrac{1}{2}m\Big(\frac{\mathrm{d}s}{\mathrm{d}t}\Big)^2 = \tfrac{1}{2}m\Delta^2\big\{(\cosh^2 u - \cos^2 v)[\dot{u}^2 + \dot{v}^2] + \cosh^2 u\cos^2 v\dot{\phi}^2\big\}. \tag{1.20}$$

The eqns of motion are therefore

$$m\Delta^2\left\{\frac{\mathrm{d}}{\mathrm{d}t}\big[((\cosh^2 u - \cos^2 v)\dot{u}\big] - \tfrac{1}{2}\sinh 2u\big(\dot{u}^2 + \dot{v}^2 + \cos^2 v\dot{\phi}^2\big)\right\} + \frac{\partial V}{\partial u} = 0$$

$$m\Delta^2\left\{\frac{\mathrm{d}}{\mathrm{d}t}\big[((\cosh^2 u - \cos^2 v)\dot{v}\big] - \tfrac{1}{2}\sin 2v\big(\dot{u}^2 + \dot{v}^2 - \cosh^2 u\dot{\phi}^2\big)\right\} + \frac{\partial V}{\partial v} = 0$$

$$m\Delta^2\left[\frac{\mathrm{d}}{\mathrm{d}t}\big(\cosh^2 u\cos^2 v\dot{\phi}\big)\right] + \frac{\partial V}{\partial\phi} = 0.$$

1.4 Lagrangian for a rigid body

Lagrangian dynamics really comes into its own for the dynamics of a rigid body – that is an object such as a spanner that contains a vast number N of particles that are so strongly coupled to each other that we may consider the distances between them to be fixed. In this approximation, the coordinates of every particle are known as soon as we have determined the six generalized coordinates that are required to specify the position and orientation of the body. Mathematically, if $\mathbf{r}_i$ is the position vector of the ith particle, $\mathbf{r}_i(q_1, \ldots, q_6)$. Newton's law of motion states that for $i = 1, \ldots, N$

$$m_i \ddot{\mathbf{r}}_i - \mathbf{F}_i = 0 \tag{1.21}$$

where $\mathbf{F}_i$ is the force on the ith particle. There are two contributions to $\mathbf{F}_i$: any external force $\mathbf{F}_i^{(\mathrm{e})}$ and the internal stress $\mathbf{f}_i$ that keeps this particle in its alloted position relative to the other particles in the body. Now we imagine instantaneously displacing the body such that $\mathbf{r}_i \to \mathbf{r}_i + \delta\mathbf{r}_i$. In view of (1.21) we have

$$\begin{aligned} 0 &= \sum_i^N (m_i \ddot{\mathbf{r}}_i - \mathbf{F}_i) \cdot \delta\mathbf{r}_i \\ &= \sum_i^N (m_i \ddot{\mathbf{r}}_i - \mathbf{F}_i^{(\mathrm{e})} - \mathbf{f}_i) \cdot \delta\mathbf{r}_i. \end{aligned} \tag{1.22}$$

The contribution $\sum_i \mathbf{f}_i \cdot \delta\mathbf{r}_i = 0$ because the internal stresses do no work (the body is rigid). So

$$0 = \sum_i^N (m_i \ddot{\mathbf{r}}_i - \mathbf{F}_i^{(\mathrm{e})}) \cdot \delta\mathbf{r}_i.$$

Now the $\delta\mathbf{r}_i$ are not all independent – they arise from a displacement of the entire body so they are functions of six independent coordinates $\delta q_1, \ldots, \delta q_6$. Hence we may write

$$0 = \sum_{i=1}^N \sum_{j=1}^6 m_i \ddot{\mathbf{r}}_i \cdot \frac{\partial \mathbf{r}_i}{\partial q_j} \delta q_j - \sum_{j=1}^6 Q_j \delta q_j, \tag{1.23a}$$

where the **generalized force Q** is defined by

$$Q_j \equiv \sum_{i=1}^N \mathbf{F}_i^{(\mathrm{e})} \cdot \frac{\partial \mathbf{r}_i}{\partial q_j}. \tag{1.23b}$$

Since the δq_j are all independent, (1.23a) implies that the coefficient of each δq_j individually vanishes. That is

$$0 = \sum_{i=1}^N m_i \ddot{\mathbf{r}}_i \cdot \frac{\partial \mathbf{r}_i}{\partial q_j} - Q_j. \tag{1.24}$$

Now we have that

$$\dot{\mathbf{r}}_i = \sum_{k=1}^{6} \frac{\partial \mathbf{r}_i}{\partial q_k}\dot{q}_k \quad \Rightarrow \quad \ddot{\mathbf{r}}_i = \sum_{k,l=1}^{6} \frac{\partial^2 \mathbf{r}_i}{\partial q_l \partial q_k}\dot{q}_l\dot{q}_k + \sum_{k=1}^{6} \frac{\partial \mathbf{r}_i}{\partial q_k}\ddot{q}_k, \tag{1.25}$$

so (1.24) can be written

$$0 = \sum_{i=1}^{N} m_i \Big(\sum_{k,l=1}^{6} \frac{\partial^2 \mathbf{r}_i}{\partial q_l \partial q_k}\dot{q}_l\dot{q}_k + \sum_{k=1}^{6} \frac{\partial \mathbf{r}_i}{\partial q_k}\ddot{q}_k \Big) \cdot \frac{\partial \mathbf{r}_i}{\partial q_j} - Q_j. \tag{1.26}$$

By the chain rule the body's k.e. is

$$T = \tfrac{1}{2} \sum_{i=1}^{N} m_i \Big| \sum_{k=1}^{6} \frac{\partial \mathbf{r}_i}{\partial q_k}\dot{q}_k \Big|^2, \tag{1.27}$$

so

$$\frac{\partial T}{\partial \dot{q}_j} = \sum_i m_i \Big(\sum_{k=1}^{6} \frac{\partial \mathbf{r}_i}{\partial q_k}\dot{q}_k \Big) \cdot \frac{\partial \mathbf{r}_i}{\partial q_j} \tag{1.28}$$

and

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t}\Big(\frac{\partial T}{\partial \dot{q}_j}\Big) = \sum_{i=1}^{N} m_i \Big[\Big(\sum_{kl} \frac{\partial^2 \mathbf{r}_i}{\partial q_l \partial q_k}\dot{q}_l\dot{q}_k + \sum_{k} \frac{\partial \mathbf{r}_i}{\partial q_k}\ddot{q}_k \Big) \cdot \frac{\partial \mathbf{r}_i}{\partial q_j} \\ + \Big(\sum_{k} \frac{\partial \mathbf{r}_i}{\partial q_k}\dot{q}_k \Big) \cdot \Big(\sum_{l} \frac{\partial^2 \mathbf{r}_i}{\partial q_l \partial q_j}\dot{q}_l \Big) \Big]. \end{aligned} \tag{1.29}$$

This expression for $(\mathrm{d}/\mathrm{d}t)(\partial T/\partial \dot{q}_j)$ contains two of the terms that appear in equation (1.26). Unfortunately its last term is unwanted. We can obtain an alternative expression for this unwanted term by calculating

$$\frac{\partial T}{\partial q_j} = \sum_{i=1}^{N} m_i \Big(\sum_{k} \frac{\partial \mathbf{r}_i}{\partial q_k}\dot{q}_k \Big) \cdot \Big(\sum_{l} \frac{\partial^2 \mathbf{r}_i}{\partial q_j \partial q_l}\dot{q}_l \Big). \tag{1.30}$$

Hence we can write (1.26) as

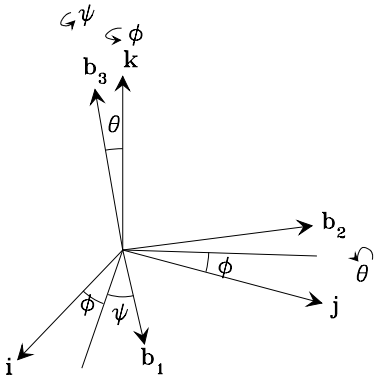
$$0 = \frac{\mathrm{d}}{\mathrm{d}t}\Big(\frac{\partial T}{\partial \dot{q}_j}\Big) - \frac{\partial T}{\partial q_j} - Q_j. \tag{1.31}$$

Now we specialize the the case in which Q_j is generated by a potential V: $Q_j = -(\partial V/\partial q_j)$. Then equation (1.31) is easily seen to the EL equation for $L = T - V$.

This analysis shows that we can obtain the equations of motion of any rigid body from the EL equations as soon as we have expressions for the body's kinetic and potential energies in terms of any set of independent coordinates. The analysis is easily extended to the case of a body that is made up of several rigid bodies that swivel or slide smoothly on one another.

Box 1: Euler Angles

To specify the orientation of a rigid body, we imagine starting with the body axes $\mathbf{b}_i$ aligned with the coordinate axes and then moving to an arbitrary orientation by compounding three rotations. We label the body axes $\mathbf{b}_1$, $\mathbf{b}_2$ and $\mathbf{b}_3$ according to whether they start parallel to $\mathbf{i}$, $\mathbf{j}$ or $\mathbf{k}$. Now we rotate by ϕ about $\mathbf{k}$, then we rotate by θ about the new position of $\mathbf{b}_2$ and finally we rotate by ψ about the new position of $\mathbf{b}_3$.



Note:

Notice that the dimensions of the generalized force Q_i are energy divided by those of q_i. The latter is frequently dimensionless (because it is an angle, for example), so generalized forces don't necessarily have dimensions of force!

Let $\rho(\mathbf{x})$ be the density of a rigid body that is rotating with angular velocity $\boldsymbol{\omega}$ about the coordinate origin. Then the body's angular momentum about the origin is

$$\begin{aligned}\mathbf{J} &= \int \mathrm{d}^3\mathbf{x}\,\rho\,\mathbf{x}\times(\boldsymbol{\omega}\times\mathbf{x}) \\ &= \int \mathrm{d}^3\mathbf{x}\,\rho\,[x^2\boldsymbol{\omega} - (\boldsymbol{\omega}\cdot\mathbf{x})\mathbf{x}].\end{aligned} \tag{1.32}$$

We rewrite this formula in tensor notation as

$$J_i = \sum_j I_{ij}\omega_j \quad \text{where} \quad I_{ij} \equiv \int \mathrm{d}^3\mathbf{x}\,\rho\,(x^2\delta_{ij} - x_i x_j). \tag{1.33}$$

Here δ_{ij} is the ij element of the identity matrix: it is zero if $i \neq j$, and unity if $i = j$. The matrix $\mathbf{I}$ defined by (1.33) is the body's **moment of inertia tensor**. Since it is a real symmetric matrix it has real eigenvalues I_i and eigenvectors $\mathbf{b}_i$. The $\mathbf{b}_i$ are called **body axes** and the I_i are called **principal moments of inertia**. When the body is rotated, the body axes rotate with it so they should be thought of as fixed within the body. According to (1.33), when the body spins such that its angular velocity lies along a body axis, its angular momentum is parallel to its angular velocity, and the proportionality constant between these two vectors is the appropriate principal moment of inertia.

The kinetic energy of our spinning body is

$$\begin{aligned} T &= \tfrac{1}{2}\int \mathrm{d}^3\mathbf{x}\,\rho\,|\boldsymbol{\omega}\times\mathbf{x}|^2 \\ &= \tfrac{1}{2}\int \mathrm{d}^3\mathbf{x}\,\rho\,\boldsymbol{\omega}\cdot[\mathbf{x}\times(\boldsymbol{\omega}\times\mathbf{x})] \\ &= \tfrac{1}{2}\boldsymbol{\omega}\cdot\mathbf{I}\cdot\boldsymbol{\omega}. \end{aligned} \tag{1.34}$$

This expression is especially simple in the body-axis frame:

$$T = \tfrac{1}{2}\sum_{i=1}^{3} I_i\omega_i^2, \qquad \text{(body-axis frame)}. \tag{1.35}$$

If all three moments of inertia are different, evaluating T from (1.35) in terms of the derivatives of Euler angles (Box 1) is tedious. So consider the case $I_1 = I_2$ of an axisymmetric body, such as a saucer. Since the Euler angle ψ is a rotation about the final position of $\mathbf{b}_3$, it is clear that $\dot\psi$ contributes $\dot\psi\mathbf{b}_3$ to $\boldsymbol{\omega}$. Since $I_1 = I_2$ we can adopt any two mutually orthogonal vectors in the body's equatorial plane as $\mathbf{b}_1$ and $\mathbf{b}_2$. So let's choose $\mathbf{b}_2$ to be the axis about which we rotated through Euler angle θ. Then $\dot\theta$ contributes $\dot\theta\mathbf{b}_2$ to $\boldsymbol{\omega}$. An increment in ϕ rotates the system about $\mathbf{k}$. This lies in the plane of $\mathbf{b}_1$ and $\mathbf{b}_3$ and is inclined at angle θ to $\mathbf{b}_3$. Hence $\dot\phi$ contributes $\dot\phi(\cos\theta\mathbf{b}_3 - \sin\theta\mathbf{b}_1)$ to $\boldsymbol{\omega}$. Adding all three contributions together to form $\boldsymbol{\omega}$ and substituting the result into (1.35) we find that the kinetic energy of an axisymmetric body is

$$T = \tfrac{1}{2}I_1(\dot\phi^2\sin^2\theta + \dot\theta^2) + \tfrac{1}{2}I_3(\dot\phi\cos\theta + \dot\psi)^2. \tag{1.36}$$

The potential energy of an axisymmetric body can depend only on θ and is usually easy to write down for any particular physical situation. Hence with (1.36) in hand the Lagrangian follows easily – see the problems.

1.5 Lagrangian for motion in an e.m. field

The simple rule $L = T - V$ does not work for a charged particle that moves in a magnetic field $\mathbf{B}$. To see this, recall that $\mathbf{B}$ does no work on the particle, so it contributes to neither T nor V. Hence it cannot appear in equations of motion that are derived from only T and V. We now show that the correct equations of motion follow from

$$L = \tfrac{1}{2}m\dot{\mathbf{x}}^2 + Q(\dot{\mathbf{x}}\cdot\mathbf{A} - \phi), \tag{1.37}$$

where Q is the particle's charge, $\mathbf{A}(\mathbf{x},t)$ is the magnetic vector potential and $\phi(\mathbf{x},t)$ is the electrostatic potential. Indeed, (1.37) gives the action as

$$S = \int \left[\tfrac{1}{2}m\dot{\mathbf{x}}^2 + Q(\dot{\mathbf{x}}\cdot\boldsymbol{A} - \phi)\right]\mathrm{d}t, \tag{1.38}$$

so the EL eqn is

$$\frac{\mathrm{d}}{\mathrm{d}t}(m\dot{\mathbf{x}} + Q\mathbf{A}) + Q\nabla(\phi - \dot{\mathbf{x}}\cdot\mathbf{A}) = 0. \tag{1.39}$$

Here the derivative w.r.t. t is along the path, so

$$\frac{\mathrm{d}\mathbf{A}}{\mathrm{d}t} = \frac{\partial \mathbf{A}}{\partial t} + (\dot{\mathbf{x}} \cdot \nabla)\mathbf{A}. \tag{1.40}$$

The partial derivative here can be combined with the $\nabla\phi$ term in (1.39) to produce the electric field $\mathbf{E} = -\nabla\phi - \partial\mathbf{A}/\partial t$. Putting all these things back into the EL eqn (1.39) yields

$$m\ddot{\mathbf{x}} = Q\big[\mathbf{E} + \nabla(\dot{\mathbf{x}} \cdot \mathbf{A}) - (\dot{\mathbf{x}} \cdot \nabla)\mathbf{A}\big]. \tag{1.41}$$

It's now straightforward to show that the last two terms on the right of (1.41) equal $\dot{\mathbf{x}} \times \mathbf{B}$ as one would hope: bearing in mind that $\nabla\dot{\mathbf{x}} = 0$ we have

$$\begin{aligned} \dot{\mathbf{x}} \times \mathbf{B} &= \dot{\mathbf{x}} \times (\nabla \times \mathbf{A}) \\ &= \nabla(\dot{\mathbf{x}} \cdot \mathbf{A}) - (\dot{\mathbf{x}} \cdot \nabla)\mathbf{A} \end{aligned}$$

Thus the EL eqn applied to the action (1.38) gives

$$m\ddot{\mathbf{x}} = Q(\mathbf{E} + \dot{\mathbf{x}} \times \mathbf{B}) \tag{1.42}$$

as required.

Note:

The action (1.38) looks rather arbitrary at this stage but is revealed to be beautifully natural when one looks at the problem in a relativistically covariant way, as one should.

1.6 Normal modes from Lagrangians

Obviously, when a system is in equilibrium all its time derivatives vanish. From the EL eqns we infer that equilibrium configurations correspond to $\partial V/\partial q_i = 0$, where q_i is any coordinate. By expanding $V(\mathbf{q})$ around the stationary point $\mathbf{q}_s$ corresponding to an equilibrium configuration and plugging the expansion into the EL eqns, one sees that the equilibrium is stable if $\mathbf{q}_s$ is a local minimum of V, and unstable otherwise.

When slightly disturbed from an stable equilibrium, the system will oscillate in a motion that can be represented as a superposition of normal modes. Lagrangians provide a relatively painless route to the frequencies and forms of these normal modes. The trick is to expand $L(\mathbf{q}, \dot{\mathbf{q}})$ in a Taylor series around the equilibrium configuration $\mathbf{q} = \mathbf{q}_s$, $\dot{\mathbf{q}} = 0$, discarding terms of higher than second order in $\delta\mathbf{q} \equiv \mathbf{q} - \mathbf{q}_s$ and its derivatives. Thus we write

$$L \simeq \tfrac{1}{2}\sum_{ij}\left(M_{ij}\delta\dot{q}_i\delta\dot{q}_j + C_{ij}\delta\dot{q}_i\delta q_j + \tfrac{1}{2}F_{ij}\delta q_i\delta q_j\right) + \sum_i A_i\delta\dot{q}_i + L_0, \tag{1.43}$$

where $\mathbf{M}$, $\mathbf{C}$, $\mathbf{F}$ and $\mathbf{A}$ are constant matrices or vectors. Since the EL eqns involve only derivatives of L, we can discard the constant L_0. It is also easy to check that the term involving $\mathbf{A}$ makes no net contribution to the equations of motion. Nor does that

involving $\mathbf{C}$ unless the latter is antisymmetric, which it won't be in practice. So we take the EL eqns to be

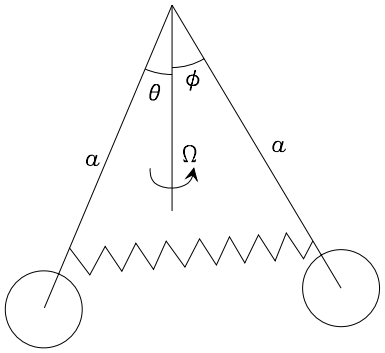
$$\sum_j M_{ij}\ddot{q}_j = \sum_j F_{ij}q_j. \tag{1.44}$$

This is easily solved by writing $\mathbf{q}(t) = \mathbf{Q}e^{\mathrm{i}\omega t}$, whence the eigenfrequencies ω are the roots of

$$\det(\mathbf{F} + \omega^2\mathbf{M}) = 0. \tag{1.45}$$

Example 2

The governor of a steam engine contains two balls of mass m that are mounted on light rods, and these are in turn attached to a vertical axis. The plane of the rods rotates at constant angular velocity Ω about the vertical axis. A spring connects the two rods in such a way that the potential energy stored in the spring is $\frac{1}{2}k$ times the square of the distance between the centres of the balls. Find a point of equlibrium and determine the frequencies of the normal modes.



Solution: Application of the cosine law to the triangle formed by the balls and their point of suspension shows that the potential energy is

$$V = -mga(\cos\phi + \cos\theta) + \tfrac{1}{2}ka^2\big[2 - 2\cos(\phi+\theta)\big]$$

Subtracting this from the kinetic energy, we find that

$$L = \tfrac{1}{2}ma^2(\dot\phi^2+\dot\theta^2)+\tfrac{1}{2}ma^2\Omega^2(\sin^2\phi+\sin^2\theta)+mga(\cos\phi+\cos\theta)-ka^2\big[1-\cos(\phi+\theta)\big].$$

By the system's symmetry, there is a point of equilibrium with $\phi = \theta = \theta_0$. Setting to zero $\partial L/\partial\theta$ evaluated at this point, we find the equlibrium point to satisfy

$$0 = ma^2\Omega^2\sin\theta_0\cos\theta_0 - mga\sin\theta_0 - ka^2\sin 2\theta_0 \quad\Rightarrow\quad \begin{cases} \sin\theta_0 = 0 \text{ or} \\ \cos\theta_0 = \dfrac{\omega_g^2}{\Omega^2 - 2\omega_s^2}, \end{cases}$$

where $\omega_g^2 \equiv g/a$, $\omega_s^2 \equiv k/m$. At (θ_0, θ_0) the second derivatives of L are

$$\frac{\partial^2 L}{\partial\theta^2} = (m\Omega^2 - k)a^2\cos 2\theta_0 - mga\cos\theta_0 \qquad \frac{\partial^2 L}{\partial\theta\partial\phi} = -ka^2\cos 2\theta_0$$
$$\frac{\partial^2 L}{\partial\phi^2} = (m\Omega^2 - k)a^2\cos 2\theta_0 - mga\cos\theta_0$$

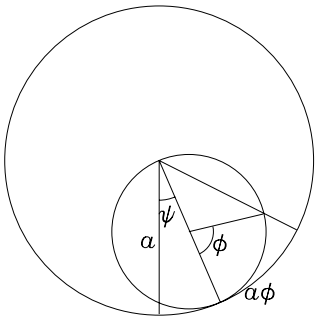
Hence the equations $\dfrac{\mathrm{d}}{\mathrm{d}t}\Big(\dfrac{\partial L}{\partial\dot\theta}\Big) = \dfrac{\partial^2 L}{\partial\theta^2}\delta\theta + \dfrac{\partial^2 L}{\partial\theta\partial\phi}\delta\phi$ etc. that govern the normal modes are

$$\begin{pmatrix} \delta\ddot\theta \\ \delta\ddot\phi \end{pmatrix} = \begin{pmatrix} x & y \\ y & x \end{pmatrix}\begin{pmatrix} \delta\theta \\ \delta\phi \end{pmatrix} \quad \text{where} \quad \begin{cases} x = (\Omega^2 - \omega_s^2)\cos 2\theta_0 - \omega_g^2\cos\theta_0 \\ y = -\omega_s^2\cos 2\theta_0 \end{cases} \tag{1.46}$$

The normal frequencies ω are given by the eigenvalues of the matrix: $\omega^2 = -x \pm y$ The lowest squared frequency, $\omega_g^2 \cos\theta_0 - \Omega^2 \cos 2\theta_0$, is negative for $\Omega^2 > \omega_g^2 \cos\theta_0 / \cos 2\theta_0$, which indicates that the system is unstable for large Ω.

Example 3

A cylinder of mass m and radius a rolls on a rough horizontal table. A second cylinder, mass m and radius $\frac{1}{2}a$ rolls inside the first. Find the normal frequencies for small disturbances from equilibrium.



Solution: Let θ be the angle through which the first cylinder has turned from equilibrium, and ϕ be the angle through which the second cylinder has rolled relative to the first (see figure). Then the line between the two centres makes an angle

$$\psi = \theta - \tfrac{1}{2}\phi \tag{1.47}$$

with the vertical. The kinetic energy of the first cylinder (translational plus rotational) is

$$T_1 = \tfrac{1}{2}m(a\dot{\theta})^2 + \tfrac{1}{2}ma^2\dot{\theta}^2. \tag{1.48}$$

The motion of the centre of the second cylinder is a compound of the leftward motion $a\dot{\theta}$ of the centre of the first cylinder, plus $\frac{1}{2}a\dot{\psi}$ tangent to the line joining the centres. The second cylinder rotates with respect to inertial space at angular velocity $\dot{\phi} + \dot{\psi}$. The total kinetic energy is therefore

$$T = m(a\dot{\theta})^2 + \tfrac{1}{2}m\left[(\tfrac{1}{2}a\dot{\psi}\cos\psi - a\dot{\theta})^2 + (\tfrac{1}{2}a\dot{\psi}\sin\psi)^2\right] + \tfrac{1}{2}m(a/2)^2(\dot{\phi}+\dot{\psi})^2. \tag{1.49}$$

The potential energy is simply

$$V = -mg\tfrac{1}{2}a\cos\psi. \tag{1.50}$$

In T, which is quadratic in the velocities, we set $\psi = 0$ and we expand V to second order in ψ, to find

$$\begin{aligned} T &= \tfrac{1}{2}ma^2(\tfrac{5}{2}\dot{\theta}^2 + \tfrac{1}{2}\dot{\theta}\dot{\phi} + \tfrac{1}{8}\dot{\phi}^2), \\ V &= \text{constant} + \tfrac{1}{4}mga(\theta - \tfrac{1}{2}\phi)^2. \end{aligned} \tag{1.51}$$

Defining $\omega_0 \equiv \sqrt{g/a}$ the equations of motion become

$$\begin{aligned} 5\ddot{\theta} + \tfrac{1}{2}\ddot{\phi} + \omega_0^2(\theta - \tfrac{1}{2}\phi) &= 0, \\ \tfrac{1}{2}\ddot{\theta} + \tfrac{1}{4}\ddot{\phi} - \tfrac{1}{2}\omega_0^2(\theta - \tfrac{1}{2}\phi) &= 0. \end{aligned} \tag{1.52}$$

The eigenfrequencies are now straightforwardly found to be $\omega = 0$ and $\omega = \sqrt{2}\omega_0$.

1.7 Noether's theorem

A **constant of motion** is any function $C(\mathbf{q}, \dot{\mathbf{q}})$ that satisfies $\mathrm{d}C/\mathrm{d}t = 0$, where $\mathbf{q}(t)$ is a solution of the eqns of motion. For example, in a 'conservative' system, energy is conserved, so $E(\mathbf{q}, \dot{\mathbf{q}})$ is a constant of motion. Finding a constant of motion is a big step towards obtaining a general solution of the equations of motion.

In general, a system with N degrees of freedom $q_1, \ldots, q_N$ admits $2N-1$ independent constants of motion. We show this by arguing that given $(\mathbf{q}, \dot{\mathbf{q}})$ at any time t, the equations of motion allow us to give the position and velocity $(\mathbf{q}^{(0)}, \dot{\mathbf{q}}^{(0)})$ at any reference time t_0. Thus $q_i^{(0)}$ or $\dot{q}_i^{(0)}$ is a function $f_\alpha(\mathbf{q}, \dot{\mathbf{q}}, t)$ with $\alpha = 1, \ldots, 2N$. On eliminating t between these $2N$ functions, we have $2N-1$ constants of motion.

It seldom happens that we can find $2N-1$ constants of motion—a rare exception is the case of motion in a Kepler potential $V \propto 1/r$. In fact it turns out that essentially complete information about solutions of the equations of motion can be extracted from N constants of motion. A system for which N constants of motion can be found is said to be **integrable**.

A theorem proved by Emmy Noether (1882–1935) provides a powerful way of extracting constants of motion from Lagrangians. Noether's theorem involves identifying a flow in configuration space that leaves L invariant. A 'flow' is an infinitesimal transformation

$$\mathbf{q} \to \mathbf{q}' = \mathbf{q} + \frac{\mathrm{d}\mathbf{q}(\mathbf{q})}{\mathrm{d}\lambda}\delta\lambda. \tag{1.53}$$

For example, the transformation $\mathbf{x} \to \mathbf{x} + \mathbf{i}\delta\lambda$, is a flow.

A flow changes the path $\mathbf{q}(t)$ into the path $\mathbf{q}'(t)$ and thus changes the value of the Lagrangian at time t by

$$\delta L = \frac{\partial L}{\partial \mathbf{q}} \cdot \delta\mathbf{q} + \frac{\partial L}{\partial \dot{\mathbf{q}}} \cdot \delta\dot{\mathbf{q}}. \tag{1.54}$$

Notice that $\delta\dot{\mathbf{q}}$ is well defined: $\delta\dot{\mathbf{q}} = \dfrac{\partial \delta\mathbf{q}}{\partial \mathbf{q}} \cdot \dot{\mathbf{q}}$.

Invariance of L just means that L takes the same value at all points that are joined by the flow. Noether's theorem states that if δL vanishes along the dynamically determined path, then

$$\frac{\mathrm{d}\mathbf{q}}{\mathrm{d}\lambda} \cdot \frac{\partial L}{\partial \dot{\mathbf{q}}} \tag{1.55}$$

is a constant of motion. Thus from the invariance of L under translation $\mathbf{x} \to \mathbf{x} + \mathbf{i}\delta\lambda$ along the x-axis, Noether's theorem deduces the constancy of

$$\mathbf{i} \cdot \frac{\partial L}{\partial \dot{\mathbf{q}}} = \frac{\partial L}{\partial \dot{x}}. \tag{1.56}$$

For a particle moving in a velocity-independent potential this is just the x-momentum $m\dot{x}$.

The proof of Noether's theorem is simple. Equating to zero equation (1.54) for δL we have

$$0 = \delta L = \frac{\partial L}{\partial \mathbf{q}} \cdot \delta\mathbf{q} + \frac{\partial L}{\partial \dot{\mathbf{q}}} \cdot \delta\dot{\mathbf{q}}. \tag{1.57}$$

Using the EL eqns to eliminate $\partial L/\partial \mathbf{q}$ this becomes

$$\begin{aligned} 0 &= \frac{\mathrm{d}}{\mathrm{d}t}\Big(\frac{\partial L}{\partial \dot{\mathbf{q}}}\Big)\cdot\delta\mathbf{q} + \frac{\partial L}{\partial \dot{\mathbf{q}}}\cdot\delta\dot{\mathbf{q}} \\ &= \frac{\mathrm{d}}{\mathrm{d}t}\Big(\frac{\partial L}{\partial \dot{\mathbf{q}}}\cdot\delta\mathbf{q}\Big), \end{aligned} \tag{1.58}$$

and the result follows on writing $\delta\mathbf{q} = (\mathrm{d}\mathbf{q}/\mathrm{d}\lambda)\delta\lambda$.

Consider the proof of conservation of angular momentum by Noether's theorem. A rotation by $\delta\theta$ about the unit vector $\hat{\mathbf{n}}$ changes $\mathbf{x}$ by $\delta\theta\hat{\mathbf{n}}\times\mathbf{x}$. So if L is invariant under this rotation, the following is a constant of motion:

$$\begin{aligned} J &\equiv \hat{\mathbf{n}}\times\mathbf{x}\cdot\frac{\partial L}{\partial \dot{\mathbf{x}}} \\ &= \hat{\mathbf{n}}\cdot\mathbf{x}\times\frac{\partial L}{\partial \dot{\mathbf{x}}}. \end{aligned} \tag{1.59}$$

For a particle moving in a velocity-independent potential this is just the component of $m\mathbf{x}\times\dot{\mathbf{x}}$ parallel to $\hat{\mathbf{n}}$.

Example 4

A certain system with coordinates x, y, and z has Lagrangian

$$L = \tfrac{1}{2}(m_1\dot{x}^2 + m_1\dot{y}^2 + m_2\dot{z}^2) + A(t)\dot{z} - \tfrac{1}{2}k\big[(x-y)^2 + (y-z)^2 + (z-x)^2\big],$$

where m_1, m_2 and k are constants and $A(t)$ is a given function of time. Obtain an expression for $A(t) - A(0)$ in terms of the values of $\dot{x}$, $\dot{y}$ and $\dot{z}$ at time t and at time zero.

Solution: L depends only on the difference between coordinates, so it is invariant under $(x, y, z) \to (x+\epsilon, y+\epsilon, z+\epsilon)$. The associated invariant is

$$\frac{\partial L}{\partial \dot{x}} + \frac{\partial L}{\partial \dot{y}} + \frac{\partial L}{\partial \dot{z}} = m_1(\dot{x}+\dot{y}) + m_2\dot{z} + A(t) \tag{1.60}$$

so

$$A(t) - A(0) = -m_1(\dot{x} - \dot{x}_0 + \dot{y} - \dot{y}_0) - m_2(\dot{z} - \dot{z}_0). \tag{1.61}$$

Here's an application to motion in a uniform magnetic field $\mathbf{B} = B\mathbf{k}$. Let's choose $\mathbf{A} = (-By, 0, 0)$. Then by (1.37) $L = \frac{1}{2}m\dot{x}^2 - QBy\dot{x}$ is invariant under two flows: (i) $\mathbf{x} \to \mathbf{x} + \mathbf{i}\delta\lambda$ and (ii) $\mathbf{x} \to \mathbf{x} + \mathbf{k}\delta\lambda$. Hence we have two invariants

$$p_x \equiv \frac{\partial L}{\partial \dot{x}} = mv_x - QBy \quad ; \quad p_z \equiv \frac{\partial L}{\partial \dot{z}} = mv_z. \tag{1.62a}$$

Choosing $\mathbf{A} = (0, Bx, 0)$ we find a third invariant for the same physical problem:

$$p_y \equiv \frac{\partial L}{\partial \dot{y}} = mv_y + QBx. \tag{1.62b}$$

The physical meaning of p_z is obvious, but what do p_x and p_y mean physically? Add them up:

$$\begin{aligned} P \equiv p_x + \mathrm{i}p_y &= m(v_x + \mathrm{i}v_y) + QB(\mathrm{i}x - y) \\ &= m\dot{\xi} + \mathrm{i}QB\xi \end{aligned} \qquad \text{where} \quad \xi \equiv x + \mathrm{i}y. \tag{1.63}$$

Solving this first-order d.e. for ξ we find

$$\xi(t) = \xi(0)\mathrm{e}^{-\mathrm{i}\omega t} + \frac{\mathrm{i}P}{m\omega}, \quad \text{where} \quad \omega \equiv \frac{QB}{m} \tag{1.64}$$

is the Larmor frequency. It is now easy to see that the real and imaginary parts of P encode the y and x coordinates of the guiding centre around which the particle gyrates.

1.8 Constraints

Sometimes it is convenient to work with more coordinates than a system has degrees of freedom. Suppose, for example, that the system consists of a dumbell of length s that is free to slide on a smooth table. This system has three degrees of freedom, namely the position of the centre of mass and the orientation of the dumbell. But we might prefer to describe the system in terms of the x and y coords of the dumbell's particles. These are not independent, but satisfy the constraint

$$(x_1 - x_2)^2 + (y_1 - y_2)^2 = s^2. \tag{1.65}$$

The dynamics of the system are obtained by extremizing the action subject to this constraint equation. Lagrange multipliers enable us to do this simply. We write the constraint equation as $C(\mathbf{q}) = 0$ and evaluate

$$\begin{aligned} 0 &= \delta S + \int \mathrm{d}t\, \lambda \delta C \\ &= \int_{t_1}^{t_2} \mathrm{d}t \sum_i \delta q_i \Big[\frac{\partial L}{\partial q_i} - \frac{\mathrm{d}}{\mathrm{d}t}\Big(\frac{\partial L}{\partial \dot{q}_i}\Big) + \lambda \frac{\partial C}{\partial q_i} \Big]. \end{aligned} \tag{1.66}$$

Here $\lambda(\mathbf{q}, t)$ is an arbitrary function. As in Lagrange's standard argument, we choose λ to ensure that the coefficient of one of the δq_i vanishes, and then conclude from the independence of the remaining q_i that their coefficients must vanish too. Hence we have for every i that

$$\frac{\mathrm{d}}{\mathrm{d}t}\Big(\frac{\partial L}{\partial \dot{q}_i}\Big) = \frac{\partial L}{\partial q_i} - \lambda \frac{\partial C}{\partial q_i}. \tag{1.67}$$

Specifically for our dumbell example, $L = \frac{1}{2}m(v_1^2 + v_2^2)$, so the equations of motion are

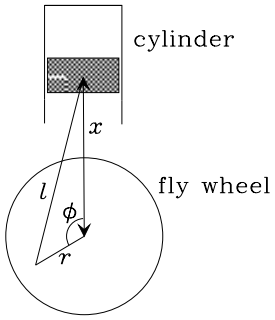
$$\begin{aligned} m\ddot{x}_1 &= -2\lambda(x_1 - x_2) & m\ddot{y}_1 &= -2\lambda(y_1 - y_2) \\ m\ddot{x}_2 &= 2\lambda(x_1 - x_2) & m\ddot{y}_2 &= 2\lambda(y_1 - y_2) \end{aligned}. \tag{1.68}$$

Adding the lower to the upper equations we obtain the equations of motion of the centre of mass: $\ddot{\mathbf{R}} = 0$, where $\mathbf{R} = \frac{1}{2}(\mathbf{r}_1 + \mathbf{r}_2)$. Dividing the top left equation by the bottom right equation and the bottom left equation by the top right equation and then subtracting the resulting equations, we obtain $\ddot{x}y - x\ddot{y} = 0$, where $x \equiv x_1 - x_2$ etc, which expresses conservation of the system's angular momentum: $\frac{\mathrm{d}}{\mathrm{d}t}(\dot{x}y - x\dot{y}) = 0$.

We shall see below that $p_i \equiv \partial L/\partial \dot{q}_i$ is the momentum 'conjugate' to q_i. Equation (1.67) expresses the rate of change of p_i as a sum of two **generalized forces**. The term $\partial L/\partial q_i$ is simply minus the gradient of the potential that would be associated with the coordinates in the absence of the constraint. This vanishes in our dumbell example. The term $-\lambda(\partial C/\partial q_i)$ describes the force associated with maintenance of the constraint. In the case of the dumbell, for example, we have that the tension T in its bar is given by

$$-T\frac{x}{s} = F_x = m\ddot{x}_1 = -2\lambda x \quad \Rightarrow \quad T = 2\lambda s. \tag{1.69}$$

Example 5



A lawn-mower engine contains a vertically mounted piston of mass m that is coupled to a fly-wheel of moment of inertia I by a light connecting rod of length l. The system has only one degree of freedom but two natural coordinates, ϕ and x. The constraint equation is

$$l^2 = x^2 + r^2 - 2rx\cos\phi. \tag{1.70}$$

The Lagrangian is

$$L = \tfrac{1}{2}I\dot{\phi}^2 + \tfrac{1}{2}m\dot{x}^2 - mgx. \tag{1.71}$$

From (1.67) the equations of motion are

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t}(m\dot{x}) &= -mgx - \lambda(2x - 2r\cos\phi) \\ \frac{\mathrm{d}}{\mathrm{d}t}(I\dot{\phi}) &= -\lambda 2rx\sin\phi. \end{aligned} \tag{1.72}$$

Eliminating λ we find that x and ϕ satisfy the d.e.

$$m\ddot{x} + \Big(\frac{\cot\phi}{x} - \frac{\mathrm{cosec}\phi}{r}\Big)I\ddot{\phi} + mg = 0. \tag{1.73}$$

Sometimes it is in principle possible to write the Lagrangian in terms of as many coordinates as the system has degrees of freedom. In such a case the constraint is called **holonomic**. Clearly, the constraint (1.65) of the dumbell is of this class, although in practice holonomic constraints will be more complex than (1.65) and correspondingly algebraically hard to eliminate.

Sometimes a constraint cannot be eliminated, *even in principle*. Such unavoidable constraints are called **non-holonomic**. The classic example of a non-holonomic constraint occurs in the problem of a rough ball moving on a rough plane. Five natural coordinates for the problem comprise the (x, y) coordinmates of the ball's centre together with three Euler angles to specify the ball's orientation. Two constraints couple the velocities of these coordinates since if the ball is moving parallel to either axis, it must be rolling and therefore the Euler angles must be incrementing in a definite way. On the other hand, it is not possible to eliminate any of these coordinates because it turns out that by rolling the ball to a chosen position, spinning it there about its point of contact with the plane and then rolling it back, one can arrange for *any* given values of the Euler angles to be associated with given values of (x, y). We can obtain equations of moton for the ball's five coordinates by a straightforward generalization of the formalism described above: we express the ball's Lagrangian (its kinetic energy) as a function of $\mathbf{q} = (x, y, \phi, \theta, \psi)$ and their derivatives and then extremize the action subject to the two constraints $C_\alpha(\mathbf{q}, \dot{\mathbf{q}})$ $(\alpha = 1, 2)$ on the positions and velocities.

2 Hamiltonian Dynamics

The Lagrangian of a dynamical system depends on $2N$ variables, the system's N coordinates and N velocities. The $2N$-dimensional space of initial conditions $(\mathbf{q}, \dot{\mathbf{q}})$ is called **phase space**. The eqns of motion allow one to determine uniquely the system's future and past from its present position in phase space. Geometrically, through every point of phase space there runs a curve along which the system evolves. These curves never intersect one another.

It turns out that $(\dot{\mathbf{q}}, \mathbf{q})$ are not the ideal coordinates for phase space. The natural coordinates are $(\mathbf{p}, \mathbf{q})$, where

$$\mathbf{p} \equiv \frac{\partial L}{\partial \dot{\mathbf{q}}} \tag{2.1}$$

is the **momentum** 'conjugate to $\mathbf{q}$'. Changing coordinates from $\dot{\mathbf{q}}$ to $\mathbf{p}$ is analogous in thermodynamics to replacing the volume V by the pressure P since $P = -(\partial U/\partial V)_S$ just as $\mathbf{p} = (\partial L/\partial \dot{\mathbf{q}})_{\mathbf{q}}$. We are replacing a variable by the gradient of some function of that variable. Transformations of this type are called **Legendre transforms** – see Box 2. When in thermodynamics we eliminate V in favour of P it is expedient to introduce a new function $H(S, P) \equiv U + PV$. So here we introduce the **Hamiltonian**

$$H(\mathbf{p}, \mathbf{q}) \equiv \mathbf{p} \cdot \dot{\mathbf{q}} - L, \tag{2.2}$$

where it is understood that $\dot{\mathbf{q}}$ is to be eliminated in favour of $\mathbf{q}$, $\mathbf{p}$, and t using equation (2.1).

Example 6

When the single degree of freedom of the lawn-mower of Example 5 is taken to be ϕ (that is, x is considered to be a function of ϕ), the momentum conjugate to ϕ is

$$p_\phi = \left(\frac{\partial L}{\partial \dot{\phi}}\right)_\phi = I\dot{\phi} + m\dot{x}\frac{\partial \dot{x}}{\partial \dot{\phi}}. \tag{2.3}$$

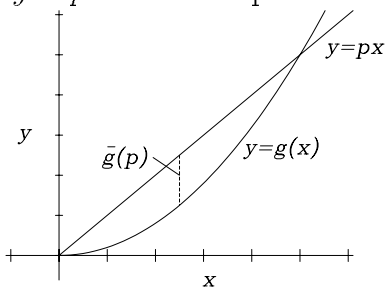
Box 2: Legendre transforms

Let $g(x)$ be a **convex function**, that is, a function such that $g''(x) > 0$. Then the **Legendre transform** $\overline{g}(p)$ of g is defined by

$$\overline{g}(p) \equiv xp - g(x) \quad \begin{array}{l}\text{where } x(p) \text{ is implicitly defined} \\ \text{as the root for given } p \text{ of}\end{array} \quad p = \frac{\partial g}{\partial x}. \tag{B2.1}$$

The convexity of g guarantees that the equation defining $x(p)$ can be solved for any p that lies between the maximum and minimum gradients of g. Thus $\overline{g}(p)$ is well defined. It is straightforward to show that Legendre transforms are invertible. In fact a Legendre transform is its own inverse: $\overline{\overline{g}}(x) = g(x)$.

It is often helpful to consider the function $\mathcal{G}(x,p) \equiv xp - g(x)$ of two independent variables (x,p). Graphically, $\mathcal{G}(x,p)$ is the vertical displacement at ordinate x between the straight line $y = px$ and the upward curving graph of $g(x)$:



The Legendre transform $\overline{g}(p)$ is the value of $\mathcal{G}$ at the point $x(p)$ at which the curve runs parallel to the line. Since

$$\frac{\partial \mathcal{G}}{\partial x} = p - \frac{\partial g}{\partial x}, \tag{B2.2}$$

$x(p)$ is the value of x which extremizes $\mathcal{G}$ for given p, as is already evident from the figure.

Differentiating the constraint eq first w.r.t. t and then w.r.t. $\dot{\phi}$ we have

$$\begin{aligned} 0 &= 2\dot{x}(x - r\cos\phi) + 2rx\sin\phi\,\dot{\phi} \\ 0 &= \frac{\partial \dot{x}}{\partial \dot{\phi}}(x - r\cos\phi) + rx\sin\phi \end{aligned} \tag{2.4}$$

Hence

$$p_\phi = \left[I + m\left(\frac{rx\sin\phi}{x - r\cos\phi}\right)^2\right]\dot{\phi}. \tag{2.5}$$

The total derivative of the Hamiltonian is

$$\begin{aligned} \mathrm{d}H &= \mathbf{p}\cdot\mathrm{d}\dot{\mathbf{q}} + \dot{\mathbf{q}}\cdot\mathrm{d}\mathbf{p} - \left(\frac{\partial L}{\partial \mathbf{q}}\right)_{\dot{\mathbf{q}},t}\cdot\mathrm{d}\mathbf{q} - \left(\frac{\partial L}{\partial \dot{\mathbf{q}}}\right)_{\mathbf{q},t}\cdot\mathrm{d}\dot{\mathbf{q}} - \left(\frac{\partial L}{\partial t}\right)_{\mathbf{q},\dot{\mathbf{q}}}\mathrm{d}t \\ &= \dot{\mathbf{q}}\cdot\mathrm{d}\mathbf{p} - \left(\frac{\partial L}{\partial \mathbf{q}}\right)_{\dot{\mathbf{q}},t}\cdot\mathrm{d}\mathbf{q} - \left(\frac{\partial L}{\partial t}\right)_{\mathbf{q},\dot{\mathbf{q}}}\mathrm{d}t, \end{aligned} \tag{2.6}$$

where the first and fourth terms cancel by (2.1). But we may also write

$$\mathrm{d}H = \left(\frac{\partial H}{\partial \mathbf{p}}\right)_{\mathbf{q},t} \cdot \mathrm{d}\mathbf{p} + \left(\frac{\partial H}{\partial \mathbf{q}}\right)_{\mathbf{p},t} \cdot \mathrm{d}\mathbf{q} + \left(\frac{\partial H}{\partial t}\right)_{\mathbf{q},\mathbf{p}} \mathrm{d}t. \tag{2.7}$$

Since equations (2.6) and (2.7) must be the same, we have

$$\dot{\mathbf{q}} = \left(\frac{\partial H}{\partial \mathbf{p}}\right)_{\mathbf{q},t} ; \quad \left(\frac{\partial H}{\partial \mathbf{q}}\right)_{\mathbf{p},t} = -\left(\frac{\partial L}{\partial \mathbf{q}}\right)_{\dot{\mathbf{q}},t} ; \quad \left(\frac{\partial H}{\partial t}\right)_{\mathbf{q},\mathbf{p}} = -\left(\frac{\partial L}{\partial t}\right)_{\mathbf{q},\dot{\mathbf{q}}}. \tag{2.8}$$

Using the EL eqns and simplifying the notation, the first two of these equations lead us to **Hamilton's equations**

$$\dot{\mathbf{q}} = \frac{\partial H}{\partial \mathbf{p}} \quad ; \quad \dot{\mathbf{p}} = -\frac{\partial H}{\partial \mathbf{q}}. \tag{2.9}$$

Along a trajectory $\big(\mathbf{q}(t), \mathbf{p}(t)\big)$, the Hamiltonian $H\big(\mathbf{q}(t), \mathbf{p}(t), t\big)$ changes at a rate

$$\frac{\mathrm{d}H}{\mathrm{d}t} = \frac{\partial H}{\partial \mathbf{q}} \cdot \dot{\mathbf{q}} + \frac{\partial H}{\partial \mathbf{p}} \cdot \dot{\mathbf{p}} + \frac{\partial H}{\partial t} = \frac{\partial H}{\partial t}. \tag{2.10}$$

Hence, if $\partial L/\partial t = 0$, it follows from equation (2.8) that the Hamiltonian is conserved along all dynamical trajectories. We can think of this as an extension of Noether's theorem: the integral H arises from the time-translation invariance of L.

Thus, for example, consider motion in the time-independent potential $V(\mathbf{x})$. If we work in Cartesian coordinates, the Lagrangian $L = \frac{1}{2}m\dot{\mathbf{x}}^2 - V(\mathbf{x})$ depends only on $\mathbf{x}$ and $\dot{\mathbf{x}}$, so $\partial L/\partial t = 0$. Hence the Hamiltonian H is conserved. The physical quantity to which H corresponds is easily found. We have $\mathbf{p} = \partial L/\partial \dot{\mathbf{x}} = m\dot{\mathbf{x}}$ and

$$\begin{aligned} H(\mathbf{x}, \mathbf{p}) &= \mathbf{p} \cdot \dot{\mathbf{x}} - L \\ &= \frac{p^2}{2m} + V(\mathbf{x}), \end{aligned} \tag{2.11}$$

which is simply the total energy $E =$ k.e. + p.e.. Thus for motion in a fixed potential the Hamiltonian is equal to the total energy.

What are $\mathbf{p}$ and H in a rotating frame? From (2.1) and (1.13) we have

$$\mathbf{p} = m(\dot{\mathbf{r}} + \boldsymbol{\omega} \times \mathbf{r}) \tag{2.12}$$

which shows that $\mathbf{p}$ isn't always the same as $m\dot{\mathbf{q}}$. In fact, here $\mathbf{p}$ is identical with mass times velocity in the underlying *inertial* frame.

Using (2.12) to eliminate $\dot{\mathbf{r}}$ from (2.2) and (1.13) we find that the Hamiltonian for a rotating frame is

$$\begin{aligned} H &= \mathbf{p} \cdot \big(\frac{\mathbf{p}}{m} - \boldsymbol{\omega} \times \mathbf{r}\big) - \frac{p^2}{2m} + V \\ &= \frac{p^2}{2m} + V - \boldsymbol{\omega} \cdot (\mathbf{r} \times \mathbf{p}). \end{aligned} \tag{2.13}$$

The first two terms sum to the energy in an underlying inertial frame, and the last term is $\boldsymbol{\omega} \cdot \mathbf{J}$, where $\mathbf{J}$ is the angular momentum. Unless V is axisymmetric [$V = V(|\boldsymbol{\omega} \times \mathbf{r}|)$], the energy in an inertial frame changes as V does work on the potential, but H is nonetheless constant.

Exercise (2):
Show that in a rotating frame we may write $H = \frac{1}{2}m|\dot{\mathbf{r}}|^2 - \frac{1}{2}m|\boldsymbol{\omega}\times\mathbf{r}|^2 + V$. What is the physical interpretation of the second term on the r.h.s?

From the Lagrangian (1.37) for non-relativistic motion in an e.m. field we find

$$\mathbf{p} = m\dot{\mathbf{x}} + Q\mathbf{A}. \tag{2.14}$$

Thus in an e.m. field $\mathbf{p}$ is not just $m\dot{\mathbf{x}}$. Problem xx explains this result by demonstrating that the e.m. field contributes $Q\mathbf{A}$ to $\mathbf{p}$. In quantum mechanics the distinction between $\mathbf{p}$ and $m\dot{\mathbf{x}}$ is of the utmost importance because it turns out that when one quantizes, it is $\mathbf{p}$ rather than $m\dot{\mathbf{x}}$ that should be replaced by $-\mathrm{i}\hbar\nabla$.

Using (2.14) in (2.2) we find H for motion in an e.m. field is

$$\begin{aligned} H &= (m\dot{\mathbf{x}} + Q\mathbf{A})\cdot\dot{\mathbf{x}} - \left[\tfrac{1}{2}m|\dot{\mathbf{x}}|^2 + Q(\dot{\mathbf{x}}\cdot\mathbf{A} - \phi)\right] \\ &= \tfrac{1}{2}m|\dot{\mathbf{x}}|^2 + Q\phi \\ &= \frac{1}{2m}|\mathbf{p} - Q\mathbf{A}|^2 + Q\phi. \end{aligned} \tag{2.15}$$

Although H is just what one would naïvely think of as the energy, when expressed in terms of $\mathbf{p}$ it looks odd.

2.1 Liouville's theorem

If we imagine releasing a bunch of dynamically identical systems from neighbouring initial conditions, then the 'phase points' describing these systems flow through phase space like a fluid. This flow is governed by Hamilton's equations (2.9). It is an incompressible flow: the 'velocity' of the fluid is $(\dot{\mathbf{p}},\dot{\mathbf{q}})$ and the divergence of this velocity is

$$\begin{aligned} \mathrm{div}(\dot{\mathbf{p}},\dot{\mathbf{q}}) &= \Big(\frac{\partial\dot{\mathbf{p}}}{\partial\mathbf{p}} + \frac{\partial\dot{\mathbf{q}}}{\partial\mathbf{q}}\Big) \\ &= \Big(-\frac{\partial^2 H}{\partial\mathbf{p}\partial\mathbf{q}} + \frac{\partial^2 H}{\partial\mathbf{q}\partial\mathbf{p}}\Big) = 0. \end{aligned}$$

The divergence-freeness of the phase flow is known as **Liouville's theorem**.

Let f be the probability density of systems in phase-space. Then conservation of probability requires that f obey the continuity equation

$$\begin{aligned} 0 &= \frac{\partial f}{\partial t} + \mathrm{div}\big((\dot{\mathbf{p}},\dot{\mathbf{q}})f\big) \\ &= \frac{\partial f}{\partial t} + \frac{\partial f}{\partial\mathbf{p}}\cdot\dot{\mathbf{p}} + \frac{\partial f}{\partial\mathbf{q}}\cdot\dot{\mathbf{q}} \\ &= \frac{\partial f}{\partial t} - \frac{\partial f}{\partial\mathbf{p}}\cdot\frac{\partial H}{\partial\mathbf{q}} + \frac{\partial f}{\partial\mathbf{q}}\cdot\frac{\partial H}{\partial\mathbf{p}} \end{aligned} \tag{2.16}$$

where Liouville's theorem has been used. The continuity equation of f in either of the last two forms is known as **Liouville's equation**.

2.2 Poisson brackets and canonical coordinates

Let $A(\mathbf{q},\mathbf{p})$ and $B(\mathbf{q},\mathbf{p})$ be any two functions of the phase-space coordinates. Then the **Poisson bracket** $[A,B]$ is defined by

$$[A,B] \equiv \frac{\partial A}{\partial \mathbf{q}} \cdot \frac{\partial B}{\partial \mathbf{p}} - \frac{\partial A}{\partial \mathbf{p}} \cdot \frac{\partial B}{\partial \mathbf{q}}. \tag{2.17}$$

It is straightforward to verify the following properties of Poisson brackets:

(i) $[A,B] = -[B,A]$ and $[A+B,C] = [A,C] + [B,C]$,

(ii) $[[A,B],C] + [[B,C],A] + [[C,A],B] = 0$ (**Jacobi identity**),

(iii) The coordinates $(\mathbf{q},\mathbf{p})$ satisfy the **canonical commutation relations**

$$[p_i,p_j] = [q_i,q_j] = 0 \quad \text{and} \quad [q_i,p_j] = \delta_{ij}. \tag{2.18}$$

(iv) Hamilton's equations may be written

$$\dot{q}_i = [q_i,H] \quad ; \quad \dot{p}_i = [p_i,H]. \tag{2.19}$$

If we write $(w_i \equiv q_i,\ w_{N+i} \equiv p_i \quad i = 1,\ldots,N)$, and define the **symplectic matrix c** by

$$c_{\alpha\beta} \equiv [w_\alpha, w_\beta] = \begin{cases} \pm 1 & \text{for } \beta = \alpha \pm N,\ 1 \le \alpha,\beta \le 2N; \\ 0 & \text{otherwise,} \end{cases} \tag{2.20a}$$

we have

$$[A,B] = \sum_{\alpha,\beta=1}^{2N} c_{\alpha\beta} \frac{\partial A}{\partial w_\alpha} \frac{\partial B}{\partial w_\beta}. \tag{2.20b}$$

Any set of $2N$ phase-space coordinates $\{W_\alpha\}$ $(\alpha = 1,\ldots,2N)$ is called a set of **canonical coordinates** if $[W_\alpha,W_\beta] = c_{\alpha\beta}$. Let $\{W_\alpha\}$ be such a set; then with equation (20b) and the chain rule we have

$$\begin{aligned} [A,B] &= \sum_{\alpha,\beta=1}^{2N} c_{\alpha\beta} \frac{\partial A}{\partial w_\alpha} \frac{\partial B}{\partial w_\beta} = \sum_{\kappa\lambda} \left(\sum_{\alpha\beta} c_{\alpha\beta} \frac{\partial W_\kappa}{\partial w_\alpha} \frac{\partial W_\lambda}{\partial w_\beta} \right) \frac{\partial A}{\partial W_\kappa} \frac{\partial B}{\partial W_\lambda} \\ &= \sum_{\kappa\lambda} [W_\kappa, W_\lambda] \frac{\partial A}{\partial W_\kappa} \frac{\partial B}{\partial W_\lambda} = \sum_{\kappa\lambda} c_{\kappa\lambda} \frac{\partial A}{\partial W_\kappa} \frac{\partial B}{\partial W_\lambda}. \end{aligned} \tag{2.21}$$

Thus the derivatives involved in the definition (2.17) of the Poisson bracket can be taken with respect to any set of canonical coordinates, just as the vector formula $\nabla \cdot \mathbf{a} = \sum_i (\partial a_i / \partial x_i)$ is valid in any Cartesian coordinate system.

The rate of change of an arbitrary canonical coordinate W_α along an orbit is

$$\dot{W}_\alpha = \sum_{\beta=1}^{2N} \frac{\partial W_\alpha}{\partial w_\beta} \dot{w}_\beta, \tag{2.22}$$

Box 3: Lorentz invariance & Symplectic structure

inertial coordinates	$\leftrightarrow$	canonical coordinates
Lorentz transformations	$\leftrightarrow$	canonical transformations
$\eta_{\mu\nu}$	$\leftrightarrow$	$c_{\alpha\beta}$
Lorentz invariant $\lvert\mathbf{x}\rvert^2$	$\leftrightarrow$	$\iint \mathrm{d}\mathbf{p}\cdot\mathrm{d}\mathbf{q}$ (Poincaré invariant)

where, as usual, $\mathbf{w} \equiv (\mathbf{q}, \mathbf{p})$. With Hamilton's equations (2.19) and equation (2.21) this becomes

$$\begin{aligned}\dot{W}_\alpha &= \sum_{\beta=1}^{2N} \frac{\partial W_\alpha}{\partial w_\beta}[w_\beta, H] = \sum_{\beta\gamma\delta} \frac{\partial W_\alpha}{\partial w_\beta} c_{\gamma\delta} \frac{\partial w_\beta}{\partial w_\gamma}\frac{\partial H}{\partial w_\delta} = \sum_{\gamma\delta} c_{\gamma\delta}\frac{\partial W_\alpha}{\partial w_\gamma}\frac{\partial H}{\partial w_\delta} \\ &= [W_\alpha, H].\end{aligned} \tag{2.23}$$

Thus Hamilton's equations (2.19) are valid in *any* canonical coordinate system.

Poisson brackets allow us to associate a one-parameter family of maps $\mathbf{B}_a$ of phase space onto itself with any function $B(\mathbf{q}, \mathbf{p})$ on phase space: from each point $(\mathbf{q}_0, \mathbf{p}_0)$ of some $(2N-1)$-dimensional surface in phase space we integrate the coupled ordinary differential equations

$$\frac{\mathrm{d}\mathbf{q}}{\mathrm{d}b} = [\mathbf{q}, B] \quad , \quad \frac{\mathrm{d}\mathbf{p}}{\mathrm{d}b} = [\mathbf{p}, B] \tag{2.24}$$

from the initial conditions $\mathbf{q}(0) = \mathbf{q}_0$, $\mathbf{p}(0) = \mathbf{p}_0$. If the initial $(2N-1)$-surface is large enough, the **integral curves** $\{\mathbf{q}(b), \mathbf{p}(b)\}$ of B reach every point of phase space. Then the map $\mathbf{B}_b$ is defined by

$$\mathbf{B}_b(\mathbf{q}(b'), \mathbf{p}(b')) = (\mathbf{q}(b+b'), \mathbf{p}(b+b')). \tag{2.25}$$

The function $B(\mathbf{q}, \mathbf{p})$ is indistinguishable from a Hamiltonian, since it satisfies Hamilton's equations (2.24), with b playing the role of the time t.

2.3 Canonical transformations*

Suppose you have a function $S(\mathbf{P}, \mathbf{q})$ of some new variables P_i, $i = 1, N$ and the regular coordinates q_i such that the equation

$$\mathbf{p} = \frac{\partial S}{\partial \mathbf{q}} \tag{2.26a}$$

* Lies beyond the syllabus

can be interpreted as defining $\mathbf{P}(\mathbf{p},\mathbf{q})$. Then it turns out that the coordinates $(\mathbf{P},\mathbf{Q})$ are canonical, where

$$\mathbf{Q} \equiv \frac{\partial S}{\partial \mathbf{P}}. \tag{2.26b}$$

That is, one may show (see Appendix I) that with these definitions, $[Q_i, Q_j] = 0$, $[Q_i, P_j] = \delta_{ij}$, $[P_i, P_j] = 0$. The transformation $(\mathbf{p},\mathbf{q}) \to (\mathbf{P},\mathbf{Q})$ is called a **canonical transformation** and S the **generating function** of the transformation.

The function that generates a canonical transformation need not be of the form $S(\mathbf{P},\mathbf{q})$; other forms are $S(\mathbf{P},\mathbf{p})$, $S(\mathbf{Q},\mathbf{q})$ and $S(\mathbf{Q},\mathbf{p})$. The generating function is always a function of one old coordinate and one new one. An entertaining transformation is generated by $S = \mathbf{Q}\cdot\mathbf{q}$:

$$\mathbf{p} = \frac{\partial S}{\partial \mathbf{q}} = \mathbf{Q} \quad ; \quad \mathbf{P} = \frac{\partial S}{\partial \mathbf{Q}} = \mathbf{q}. \tag{2.27}$$

Canonical transformations are closely connected to the one-parameter maps introduced above. To see this consider functions S of the form

$$S = \mathbf{P}\cdot\mathbf{q} + s(\mathbf{P},\mathbf{q})\delta u, \tag{2.28}$$

where $\delta u \ll 1$. For S of this form we have

$$\begin{aligned} &\mathbf{Q} = \mathbf{q} + \frac{\partial s}{\partial \mathbf{P}}\delta u \quad ; \quad \mathbf{p} = \mathbf{P} + \frac{\partial s}{\partial \mathbf{q}}\delta u \quad \Rightarrow \\ &\mathbf{P} = \mathbf{p} - \frac{\partial s}{\partial \mathbf{q}}\delta u. \end{aligned} \tag{2.29}$$

Thus $S = \mathbf{P}\cdot\mathbf{q}$ generates the identity transformation $\mathbf{P} = \mathbf{p}$, $\mathbf{Q} = \mathbf{q}$. Moreover,

$$\begin{aligned} \frac{\mathbf{Q}-\mathbf{q}}{\delta u} &= \frac{\partial s}{\partial \mathbf{P}} \\ \frac{\mathbf{P}-\mathbf{p}}{\delta u} &= -\frac{\partial s}{\partial \mathbf{q}} \end{aligned} \tag{2.30}$$

In the limit $\delta u \to 0$ we can identify $\mathbf{P}$ with $\mathbf{p}$ on the right, and these equations become

$$\frac{\mathrm{d}\mathbf{q}}{\mathrm{d}u} = [\mathbf{q}, s] \quad ; \quad \frac{\mathrm{d}\mathbf{p}}{\mathrm{d}u} = [\mathbf{p}, s], \tag{2.31}$$

which is identical with (2.24). Thus canonical transformations generated by functions of the form (2.28) may be thought of as infinitesimal canonical maps.

There is no fundamental difference between a map and a coordinate transformation: every map generates a coordinate transformation and every transformation a map since one can treat changed coordinates as new numbers describing an old point (a coordinate change), or as old numbers describing a new point (a mapping).

2.4 Point transformations*

If $(Q_i(\mathbf{q}),\ i = 1, \ldots, N)$ are any N independent functions of the generalized coordinates $\mathbf{q}$, then by equation (2.1) we obtain the new momenta $P_i = (\partial L/\partial \dot{Q}_i)$ by expressing the Lagrangian as a function $L(\mathbf{Q}, \dot{\mathbf{Q}})$ of the Q_i and their time derivatives. The coordinate change $(\mathbf{q}, \mathbf{p}) \to (\mathbf{Q}, \mathbf{P})$ is called a **point transformation**, because the new coordinates are functions only of the old. It is straightforward to show that the new coordinates are canonical, by evaluating their Poisson brackets.

The importance of these results is that it is often convenient to work in curvilinear coordinates $\mathbf{Q}$ and derive the corresponding momenta $\mathbf{P} = (\partial L/\partial \dot{\mathbf{Q}})$. Since the coordinates $(\mathbf{Q}, \mathbf{P})$ are canonical, the Poisson bracket (2.17) can be equally well evaluated by taking derivatives with respect to $\mathbf{Q}$ and $\mathbf{P}$ as with respect to $\mathbf{q}$ and $\mathbf{p}$. Hence all curvilinear coordinates have equal status in Hamiltonian mechanics.

Example 7

A particle of mass m and charge Q_1 moves in a bound orbit around a fixed charge Q_2 in the plane perpendicular to a constant magnetic field B. Determine the system's Hamiltonian in polar coordinates (r, θ) on the orbital plane. Hence show that $mr^2\dot{\theta} + \frac{1}{2}Q_1 r^2 B$ is constant on the orbit.

Solution: The vector potential can be written $\mathbf{A} = \frac{1}{2}rB\mathbf{e}_\theta$. From (1.37) the Lagrangian is

$$L = \tfrac{1}{2}m(\dot{r}^2 + r^2\dot{\theta}^2) + Q_1\left(r\dot{\theta}\tfrac{1}{2}rB - \frac{Q_2}{4\pi\epsilon_0 r}\right), \tag{2.32}$$

so the momenta are

$$p_r = m\dot{r} \quad p_\theta = mr^2\dot{\theta} + \tfrac{1}{2}Q_1 r^2 B \tag{2.33}$$

Finally, the Hamiltonian is

$$H(p_r, p_\theta, r, \theta) = \frac{p_r^2}{2m} + \frac{(p_\theta - \frac{1}{2}Q_1 B r^2)^2}{2mr^2} + \frac{Q_1 Q_2}{4\pi\epsilon_0 r}.$$

The constancy of p_θ follows because H is independent of θ. Notice that (2.33) is *not* simply the translation into polar coordinates of equation (2.15), which gives H in Cartsesian coordinates: when translating H from one coordinate system to another one *must* pass through the Lagrangian.

2.5 Phase-space volumes*

Often, for example when doing statistical mechanics, one needs a credible definition of 'phase-space volume'. If one is using Cartesian coordinates to describe a system of n particles of mass m_i, it is natural to take the volume element to be $\mathrm{d}\tau = \prod_i^n (m_i^3 \mathrm{d}^3\mathbf{x}_i \mathrm{d}^3\mathbf{v}_i)$. But it isn't immediately obvious what to use for $\mathrm{d}\tau$ in a more complex case. In particular, if one decided to describe the system of particles by some

* Lies beyond the syllabus

curvilinear coordinates $\mathbf{q}(\mathbf{x})$ and their conjugate momenta $\mathbf{p}$, one would expect $\mathrm{d}\tau$ to be of the form

$$\mathrm{d}\tau = \prod_{i=1}^{n} \left(\frac{\partial(m_i \mathbf{v}_i, \mathbf{x}_i)}{\partial(\mathbf{p}_i, \mathbf{q}_i)} \mathrm{d}^3\mathbf{p}_i \mathrm{d}^3\mathbf{q}_i \right). \tag{2.34}$$

One of the most beautiful and useful results in the subject is that the Jacobian here is just one. In fact, the Jacobian between *any* pair of canonical coordinates is always one. That is, the volume of an arbitrary region is

$$V = \iint_{\mathcal{V}} \mathrm{d}^N\mathbf{p}\mathrm{d}^N\mathbf{q} = \iint_{\mathcal{V}} \mathrm{d}^N\mathbf{P}\mathrm{d}^N\mathbf{Q}, \tag{2.35}$$

where $(\mathbf{p}, \mathbf{q})$ and $(\mathbf{P}, \mathbf{Q})$ are *any* canonical coordinates.

2.6 Hamilton-Jacobi Equation*

Suppose we could find N constants of motion $I_1, \ldots, I_N$. And suppose it were possible to find a system of canonical coordinates $(\mathbf{P}, \mathbf{Q})$ such that $P_i = I_i$ etc. Then the equations of motion for the P's would be trivial,

$$\begin{aligned} 0 = \dot{P}_i &= [P_i, H] \\ &= -\frac{\partial H}{\partial Q_i}. \end{aligned} \tag{2.36}$$

and would demonstrate that $H(\mathbf{P})$ would be independent of the Q's. This last observation would allow us to solve the equations of motion for the Q's: we would have

$$\dot{Q}_i = \frac{\partial H}{\partial P_i} \equiv \omega_i, \quad \text{a constant} \quad \Rightarrow \quad Q_i(t) = Q_i(0) + \omega_i t. \tag{2.37}$$

So everything would lie at our feet if we could find N constants of the motion and could embed these as the 'momenta' of a system of canonical coordinates.[2] The magic coordinates $\mathbf{P} \equiv \mathbf{I}$ and $\mathbf{Q}$ are called **action-angle** coordinates, the I's being the actions and the Q's the angles.

Let $S(\mathbf{I}, \mathbf{q})$ be the generating function of the transformation between regular coordinates $(\mathbf{p}, \mathbf{q})$ and action-angle coordinates. Then we can use this to eliminate $\mathbf{p} = \partial S/\partial \mathbf{q}$ from H, expressing H as a function of $(\mathbf{I}, \mathbf{q})$:

$$\widetilde{H}(\mathbf{I}, \mathbf{q}) \equiv H\Big(\frac{\partial S}{\partial \mathbf{q}}, \mathbf{q}\Big). \tag{2.38}$$

By moving on an orbit we can vary the q_i pretty much at will while holding constant the I_i. As we vary the q_i in this way H must remain constant at the energy E of the

* Lies beyond the syllabus

[2] Notice that to be able to embed the I's as a set of momenta, we require $[I_i, I_j] = 0$; functions satisfying this condition are said to be 'in involution'.

orbit in question. This suggests that we investigate the non-linear partial differential equation

$$H\Big(\frac{\partial S}{\partial \mathbf{q}}, \mathbf{q}\Big) = E, \qquad \textbf{(Hamilton-Jacobi equation)}. \tag{2.39}$$

If we can solve this equation, we identify the arbitrary constants on which the solution $S(\mathbf{q})$ depends with functions of the constants of motion I_i. For example, the H-J eqn for a free particle moving in two dimensions is

$$\frac{|\nabla S|^2}{2m} = E \tag{2.40}$$

We write $S(\mathbf{x}) = S_x(x) + S_y(y)$ and solve (2.40) by separation of variables:

$$\text{constant} \equiv I_x = \Big(\frac{\partial S}{\partial x}\Big)^2 = 2mE - \Big(\frac{\partial S}{\partial y}\Big)^2 \equiv I_y. \tag{2.41}$$

This example is very tame, but the technique works also for more complicated Hamiltonians that cannot be solved by other means.

The similarity between the H-J eqn and the time-independent Schrödinger eqn is obvious.

2.7 The Hamiltonian principle of least action*

The principle of least action

$$\delta S = 0 \tag{2.42}$$

is concerned with paths $\mathbf{q}(t)$ through coordinate space. We can derive classical mechanics from another, closely related, variational principle which involves paths $\big(\mathbf{p}(t), \mathbf{q}(t)\big)$ through phase space rather than coordinate space. This principle is that the path actually followed between $(t_\mathrm{i}, \mathbf{q}_\mathrm{i})$ and $(t_\mathrm{f}, \mathbf{q}_\mathrm{f})$ is that for which

$$\delta S = 0 \quad \text{where} \quad S \equiv \int \mathbf{p}\cdot \mathrm{d}\mathbf{q} - H(\mathbf{p},\mathbf{q})\,\mathrm{d}t. \tag{2.43}$$

Here the path of integration runs between $(t_\mathrm{i}, \mathbf{q}_\mathrm{i})$ and $(t_\mathrm{f}, \mathbf{q}_\mathrm{f})$ – neither $\mathbf{p}(t_\mathrm{i})$ nor $\mathbf{p}(t_\mathrm{f})$ is constrained. Showing that this principle yields Hamilton's equations (2.9) is easy:

$$\begin{aligned} \delta S &= \int \Big(\delta\mathbf{p}\cdot\dot{\mathbf{q}} + \mathbf{p}\cdot\delta\dot{\mathbf{q}} - \frac{\partial H}{\partial \mathbf{p}}\cdot\delta\mathbf{p} - \frac{\partial H}{\partial \mathbf{q}}\cdot\delta\mathbf{q}\Big)\mathrm{d}t \\ &= \int \Big[\Big(\dot{\mathbf{q}} - \frac{\partial H}{\partial \mathbf{p}}\Big)\cdot\delta\mathbf{p} - \Big(\dot{\mathbf{p}} + \frac{\partial H}{\partial \mathbf{q}}\Big)\cdot\delta\mathbf{q}\Big]\mathrm{d}t + \big[\mathbf{p}\cdot\delta\mathbf{q}\big]_{t_\mathrm{i}}^{t_\mathrm{f}}. \end{aligned} \tag{2.44}$$

Since $\delta\mathbf{q}$ vanishes at t_i and t_f by hypothesis, the final term in (2.44) vanishes. Then, with $\delta\mathbf{p}$ and $\delta\mathbf{q}$ subject to arbitrary variation, it is clear that $\delta S = 0$ only if the contents

* Lies beyond the syllabus

of the pairs of large round brackets in (2.44) vanish. But the vanishing of brackets is precisely the content of Hamilton's equations.

Notice that a very remarkable thing is being done with the variational principle (2.43): we are treating $\mathbf{p}$ as quite independent of the value of $\dot{\mathbf{q}}$ along the path. This makes perfectly good sense from the point of view of phase-space geometry, but it makes a mockery of our original definition (2.1) of $\mathbf{p}$. This definition is recovered for the true path as a consequence of the variational principle (2.43):

$$\begin{aligned}\dot{\mathbf{q}} &= \frac{\partial H}{\partial \mathbf{p}} = \frac{\partial}{\partial \mathbf{p}}(\mathbf{p}\cdot\dot{\mathbf{q}} - L) \\ &= \dot{\mathbf{q}} + \Big(\mathbf{p} - \frac{\partial L}{\partial \dot{\mathbf{q}}}\Big)\cdot\frac{\partial \dot{\mathbf{q}}}{\partial \mathbf{p}}.\end{aligned} \tag{2.45}$$

Recall that we introduced H as $\mathbf{p}\cdot\dot{\mathbf{q}} - L$, with $\dot{\mathbf{q}}$ eliminated in favour of $\mathbf{p}$. Now that we are treating $\mathbf{p}$ as independent of $\dot{\mathbf{q}}$, $\mathbf{p}\cdot\dot{\mathbf{q}} - H$ becomes a quantity different from L; indeed, L depends only on the projection of a phase-space path $\big(\mathbf{p}(t), \mathbf{q}(t)\big)$ onto configuration space, while $\mathbf{p}\cdot\dot{\mathbf{q}} - H$ depends on $\mathbf{p}(t)$ as well as $\mathbf{q}(t)$. Thus the action principle (2.43) is entirely different from (2.42), although the extremal values of the two integrals are the same because along the extremal path $\mathbf{p} = \partial L/\partial\dot{\mathbf{q}}$.

In Appendix II (2.43) is derived from the Schrödinger equation. The basic idea is simple: from the Schrödinger equation we calculate the quantum amplitude to get from $(t_\mathrm{i}, \mathbf{q}_\mathrm{i})$ to $(t_\mathrm{f}, \mathbf{q}_\mathrm{f})$ and show that it can be expressed as a sum over all possible paths between these events of amplitudes proportional to $e^{\mathrm{i}S/\hbar}$, where S is defined by (2.43). Then we argue that the only paths which make a net contribution to the overall amplitude are those whose values of S lie within $\sim\hbar$ of a stationary value, since the contributions of other paths are cancelled by oppositely signed contributions from neighbouring paths. Thus the overall amplitude is dominated by contributions from paths that lie within $\sim\hbar$ of the classical, extremizing, path, and from a macroscopic point of view these paths are identical with the classical path.

Appendix I: Proof that generating functions generate canonical transformations

We prove that given $S(\mathbf{q}, \mathbf{P})$, $\mathbf{P}$ and $\mathbf{Q} \equiv \partial S/\partial\mathbf{P}$ satisfy the canonical commutation relations. From the chain rule we have that

$$\begin{aligned}\frac{\partial}{\partial \mathbf{p}}\Big)_{\mathbf{q}} &= \Big(\frac{\partial \mathbf{P}}{\partial \mathbf{p}}\Big)_{\mathbf{q}}\cdot\frac{\partial}{\partial \mathbf{P}}\Big)_{\mathbf{q}} \\ \frac{\partial}{\partial \mathbf{q}}\Big)_{\mathbf{p}} &= \frac{\partial}{\partial \mathbf{q}}\Big)_{\mathbf{P}} + \Big(\frac{\partial \mathbf{P}}{\partial \mathbf{q}}\Big)_{\mathbf{p}}\cdot\frac{\partial}{\partial \mathbf{P}}\Big)_{\mathbf{q}}.\end{aligned} \tag{AI.1}$$

Applying these formulae to p_i and using $\partial p_i/\partial\mathbf{P} = \partial^2 S/\partial q_i\partial\mathbf{P} = \partial\mathbf{Q}/\partial q_i$ yields

$$\begin{aligned}\delta_{ij} &= \Big(\frac{\partial \mathbf{P}}{\partial p_j}\Big)_{\mathbf{q}}\cdot\Big(\frac{\partial \mathbf{Q}}{\partial q_i}\Big)_{\mathbf{q}} \\ -\Big(\frac{\partial p_i}{\partial q_j}\Big)_{\mathbf{P}} &= \Big(\frac{\partial \mathbf{P}}{\partial q_j}\Big)_{\mathbf{p}}\cdot\Big(\frac{\partial \mathbf{Q}}{\partial q_i}\Big)_{\mathbf{q}}\end{aligned} \tag{AI.2}$$

Multiplying these equations together and summing over j we find

$$\begin{aligned}\sum_{kl}\left(\frac{\partial Q_k}{\partial q_i}\right)_{\mathbf{q}}\left(\frac{\partial Q_l}{\partial q_{i'}}\right)_{\mathbf{q}}[P_k,P_l] &= -\left(\frac{\partial p_i}{\partial q_{i'}}\right)_{\mathbf{P}}+\left(\frac{\partial p_{i'}}{\partial q_i}\right)_{\mathbf{P}}\\ &= -\frac{\partial^2 S}{\partial q_{i'}\partial q_i}+\frac{\partial^2 S}{\partial q_i\partial q_{i'}}=0.\end{aligned}\tag{AI.3}$$

Since the matrix $\partial Q_k/\partial q_i$ has an inverse by (AI.2), this shows that $[P_k,P_l]=0$.

Working again from equations (AI.1) we have

$$\begin{aligned}[Q_i,P_j] &= \left(\frac{\partial Q_i}{\partial \mathbf{q}}\right)_{\mathbf{p}}\cdot\left(\frac{\partial P_j}{\partial \mathbf{p}}\right)_{\mathbf{q}}-\left(\frac{\partial Q_i}{\partial \mathbf{p}}\right)_{\mathbf{q}}\cdot\left(\frac{\partial P_j}{\partial \mathbf{q}}\right)_{\mathbf{p}}\\ &= \left[\left(\frac{\partial Q_i}{\partial \mathbf{q}}\right)_{\mathbf{P}}+\left(\frac{\partial Q_i}{\partial \mathbf{P}}\right)_{\mathbf{q}}\cdot\left(\frac{\partial \mathbf{P}}{\partial \mathbf{q}}\right)_{\mathbf{p}}\right]\cdot\left(\frac{\partial P_j}{\partial \mathbf{p}}\right)_{\mathbf{q}}\\ &\qquad -\left(\frac{\partial Q_i}{\partial \mathbf{P}}\right)_{\mathbf{q}}\cdot\left(\frac{\partial \mathbf{P}}{\partial \mathbf{p}}\right)_{\mathbf{q}}\cdot\left(\frac{\partial P_j}{\partial \mathbf{q}}\right)_{\mathbf{p}}\\ &= \left(\frac{\partial Q_i}{\partial \mathbf{q}}\right)_{\mathbf{P}}\cdot\left(\frac{\partial P_j}{\partial \mathbf{p}}\right)_{\mathbf{q}}+\left(\frac{\partial Q_i}{\partial \mathbf{P}}\right)_{\mathbf{q}}\cdot[\mathbf{P},P_j]\\ &= \frac{\partial^2 S}{\partial P_i\partial \mathbf{q}}\cdot\left(\frac{\partial P_j}{\partial \mathbf{p}}\right)_{\mathbf{q}}\\ &= \left(\frac{\partial \mathbf{p}}{\partial P_i}\right)_{\mathbf{q}}\cdot\left(\frac{\partial P_j}{\partial \mathbf{p}}\right)_{\mathbf{q}}=\delta_{ij}.\end{aligned}\tag{AI.4}$$

Similarly,

$$\begin{aligned}[Q_i,Q_j] &= \left[\left(\frac{\partial Q_i}{\partial \mathbf{q}}\right)_{\mathbf{P}}+\left(\frac{\partial Q_i}{\partial \mathbf{P}}\right)_{\mathbf{q}}\cdot\left(\frac{\partial \mathbf{P}}{\partial \mathbf{q}}\right)_{\mathbf{p}}\right]\cdot\left(\frac{\partial Q_j}{\partial \mathbf{p}}\right)_{\mathbf{q}}\\ &\qquad -\left(\frac{\partial Q_i}{\partial \mathbf{P}}\right)_{\mathbf{q}}\cdot\left(\frac{\partial \mathbf{P}}{\partial \mathbf{p}}\right)_{\mathbf{q}}\cdot\left(\frac{\partial Q_j}{\partial \mathbf{q}}\right)_{\mathbf{p}}\\ &= \left(\frac{\partial Q_i}{\partial \mathbf{q}}\right)_{\mathbf{P}}\cdot\left(\frac{\partial Q_j}{\partial \mathbf{p}}\right)_{\mathbf{q}}+\left(\frac{\partial Q_i}{\partial \mathbf{P}}\right)_{\mathbf{q}}\cdot[\mathbf{P},Q_j]\\ &= \left(\frac{\partial Q_i}{\partial \mathbf{q}}\right)_{\mathbf{P}}\cdot\left(\frac{\partial Q_j}{\partial \mathbf{p}}\right)_{\mathbf{q}}-\left(\frac{\partial Q_i}{\partial P_j}\right)_{\mathbf{q}}\\ &= \sum_k\frac{\partial^2 S}{\partial P_i\partial q_k}\left(\frac{\partial Q_j}{\partial \mathbf{P}}\right)_{\mathbf{q}}\cdot\left(\frac{\partial \mathbf{P}}{\partial p_k}\right)_{\mathbf{q}}-\left(\frac{\partial Q_i}{\partial P_j}\right)_{\mathbf{q}}.\end{aligned}$$

But $\left.\dfrac{\partial p_k}{\partial \mathbf{P}}\right)_{\mathbf{q}} = \dfrac{\partial^2 S}{\partial q_k \partial \mathbf{P}}$, so

$$\begin{aligned}[Q_i, Q_j] &= \sum_k \left(\frac{\partial Q_j}{\partial P_l}\right)_{\mathbf{q}} \left(\frac{\partial P_l}{\partial p_k}\right)_{\mathbf{q}} \left(\frac{\partial p_k}{\partial P_i}\right)_{\mathbf{q}} - \left(\frac{\partial Q_i}{\partial P_j}\right)_{\mathbf{q}} \\ &= \frac{\partial Q_j}{\partial P_i} - \frac{\partial Q_i}{\partial P_j} \\ &= \frac{\partial^2 S}{\partial P_i \partial P_j} - \frac{\partial^2 S}{\partial P_j \partial P_i} = 0. \qquad \triangleleft\end{aligned} \tag{AI.5}$$

Appendix II: Derivation of (2.43) from the Schrödinger equation

We start by finding the amplitude A_{12} to get from $(t_1, \mathbf{q}_1)$ to $(t_2, \mathbf{q}_2)$, where the interval $t_2 - t_1$ is small. In Dirac's notation, this amplitude is

$$A_{12} = \langle \mathbf{q}_2 | \psi, t_2 \rangle, \tag{AII.1}$$

where $|\psi, t_2\rangle$ is the ket into which $|\mathbf{q}_1\rangle$ has evolved at t_2. In other words, $|\psi, t_2\rangle$ is the solution of the time-dependent Schrödinger equation (TDSE) for initial condition $|\psi, t_1\rangle = |\mathbf{q}_1\rangle$. This is

$$|\psi, t_2\rangle = e^{-\mathrm{i}\hat{H}(t_2 - t_1)/\hbar} |\mathbf{q}_1\rangle. \tag{AII.2}$$

Here the exponential is the operator with the same eigen-kets $|E_n\rangle$ as the Hamiltonian $\hat{H}$, and eigenvalues equal to $e^{\mathrm{i}E_n(t_2-t_1)/\hbar}$, where the E_n are the eigen-values of $\hat{H}$. That is,

$$e^{\mathrm{i}\hat{H}(t_2-t_1)/\hbar} \equiv \sum_n |E_n\rangle e^{-\mathrm{i}E_n(t_2-t_1)/\hbar} \langle E_n|. \tag{AII.3}$$

(To prove that (AII.2) satisfies the TDSE, just substitute (AII.3) into (AII.2) and differentiate w.r.t. t_2.) Our amplitude can now be written

$$\begin{aligned}A_{12} &= \langle \mathbf{q}_2 | e^{-\mathrm{i}\hat{H}(t_2-t_1)/\hbar} | \mathbf{q}_1 \rangle \\ &= \int \mathrm{d}^3\mathbf{p} \langle \mathbf{q}_2 | \mathbf{p} \rangle \langle \mathbf{p} | e^{-\mathrm{i}\hat{H}(t_2-t_1)/\hbar} | \mathbf{q}_1 \rangle,\end{aligned} \tag{AII.4}$$

where use has been made of the fact that $\int \mathrm{d}^3\mathbf{p}\, |\mathbf{p}\rangle\langle\mathbf{p}|$ is just the identity operator since the states $|\mathbf{p}\rangle$ of well-defined momentum form a complete set.

$\hat{H}$ and thus the function of it appearing in (AII.4) is a function of the operators $\hat{\mathbf{p}}$ and $\hat{\mathbf{q}}$. Let's assume that every $\hat{\mathbf{p}}$ has been positioned to the left of every $\hat{\mathbf{q}}$. Then every $\hat{\mathbf{p}}$ can be considered to act to the left and be replaced by its eigen-value $\mathbf{p}$, while every $\hat{\mathbf{q}}$ acts similarly to the right. So the complex number $\langle \mathbf{p} | e^{-\mathrm{i}\hat{H}(t_2-t_1)/\hbar} | \mathbf{q}_1 \rangle$ becomes simply

$$e^{-\mathrm{i}H(t_2-t_1)/\hbar} \langle \mathbf{p} | \mathbf{q}_1 \rangle = e^{-\mathrm{i}H(t_2-t_1)/\hbar} \frac{e^{-\mathrm{i}\mathbf{p}\cdot\mathbf{q}_1/\hbar}}{\sqrt{2\pi\hbar}}, \tag{AII.5}$$

where H is the classical Hamiltonian evaluated at the classical phase-space point $(\mathbf{p},\mathbf{q})$ and we have used the fact that $\langle \mathbf{p}|\mathbf{q}_1\rangle$ is just the complex conjugate of the wave-function of a particle of well-defined momentum $\mathbf{p}$. When we insert (AII.5) into (AII.4) and similarly replace $\langle \mathbf{q}_2|\mathbf{p}\rangle$ by a plane wave, we find

$$A_{12} = \frac{1}{h}\int \mathrm{d}^3\mathbf{p}\, \exp\Big[\frac{\mathrm{i}}{\hbar}\Big(\mathbf{p}\cdot(\mathbf{q}_2-\mathbf{q}_1) - H(t_2-t_1)\Big)\Big]. \qquad \text{(AII.6)}$$

Equation (AII.6) for the amplitude to get from one event to another is only valid for infinitesimal t_2-t_1. There are two issues: (i) $\hat{H}$ may be time-dependent; (ii) for finite τ the operator $e^{-\mathrm{i}\hat{H}\tau} = 1 - \mathrm{i}\hat{H}\tau + \frac{1}{2!}(\hat{H}\tau)^2 + \cdots$ involves high powers of $\hat{H}$ and so many reversals of the order of the operators $\hat{\mathbf{p}}$ and $\hat{\mathbf{q}}$ will be required to ensure that the $\hat{\mathbf{p}}$'s are to the left of all $\hat{\mathbf{q}}$'s. In view of these objections we use (AII.6) only for small t_2-t_1. Given two widely separated events $(t_\mathrm{i},\mathbf{q}_\mathrm{i})$ and $(t_\mathrm{f},\mathbf{q}_\mathrm{f})$, we express the amplitude to pass between them by a particular path $\mathbf{q}_\mathrm{i}\to\mathbf{q}_1\to\ldots\to\mathbf{q}_\mathrm{f}$ as the product

$$A_{\mathrm{i}1}A_{12}\times\cdots\times A_{m,\mathrm{f}} \qquad \text{(AII.7))}$$

of m amplitudes of the form (AII.6) over small intervals (t_{j-1},t_j). We then obtain the amplitude to pass between $(t_\mathrm{i},\mathbf{q}_\mathrm{i})$ and $(t_\mathrm{f},\mathbf{q}_\mathrm{f})$ by *any* path by summing (AII.7) over all values of the intermediate positions $\mathbf{q}_j$. The final amplitude is

$$\begin{aligned} A_{\mathrm{if}} &= \lim_{m\to\infty}\frac{1}{h^{3m}}\int\prod_j^m(\mathrm{d}^3\mathbf{p}_j\mathrm{d}^3\mathbf{q}_j)\,\exp\Big[\frac{\mathrm{i}}{\hbar}\sum_k^m\Big(\mathbf{p}_k\cdot(\mathbf{q}_{k+1}-\mathbf{q}_k) - H(t_{k+1}-t_k)\Big)\Big] \\ &= \text{constant}\times\int\mathcal{D}\mathbf{p}\mathcal{D}\mathbf{q}\,\exp\Big[\frac{\mathrm{i}}{\hbar}\int\Big(\mathbf{p}\cdot\mathrm{d}\mathbf{q} - H\,\mathrm{d}t\Big)\Big]. \end{aligned} \qquad \text{(AII.8)}$$

Here the symbol $\mathcal{D}\mathbf{p}\mathcal{D}\mathbf{q}$ means one is to sum the integrand over all paths $\big(\mathbf{p}(t),\mathbf{q}(t)\big)$ which pass through $(t_\mathrm{i},\mathbf{q}_\mathrm{i})$ and $(t_\mathrm{f},\mathbf{q}_\mathrm{f})$.

Thus, as claimed in §3.3, the amplitude to get from $(t_\mathrm{i},\mathbf{q}_\mathrm{i})$ to $(t_\mathrm{f},\mathbf{q}_\mathrm{f})$ is a sum over all paths of $\mathrm{e}^{\mathrm{i}S/\hbar}$, where S is the classical action for that path. When $|S|\gg\hbar$ the contributions from non-classical paths that do not extremize S will cancel each other out to high precision.

Exercise (3):

In (AII.8) replace H with $\frac{1}{2}\mathbf{p}^2/m + V(\mathbf{q})$ and $\mathrm{d}\mathbf{q}$ by $\dot{\mathbf{q}}\mathrm{d}t$. Then do the integration over every $\mathbf{p}_j$ by completing the square and using $\int_{-\infty}^{\infty}e^{-x^2}\mathrm{d}x = \sqrt{\pi}$. Explain the relation of the resulting expression for A_{if} to the Lagrangian principle of least action.