Part II Classical Field Theory

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Preface

Classical field theory deals with the general idea of a quantity that is a function of time and space, which can be used to describe wave-like physical phenomena such as sound and light, or other continuous phenomena such as fluid flow. The word 'classical' is here used in the sense 'not quantum mechanical'. We shall define a field to be classical if it satisfies the following criteria:

1. The state of the field at a given time is represented by furnishing, for each point in space, a finite set of numbers (e.g. a single real number or a tensor or a spinor, depending on the type of field).
2. The field can in principle be observed without disturbing it.

By contrast, a quantum field would be described by furnishing at each point in space a set of operators not numbers, and it could not in general be observed without disturbing it. It is important to maintain a tight grip on terminology here, because in many textbooks the equations described in this chapter are first introduced in the context of quantum mechanics. However I believe it is better to become acquainted with these fields in their classical guise first, and then quantise them afterwards.

In the whole of this book up to and including this chapter, all fields mentioned are classical fields. The electromagnetic field has been shown to be a tensor field. We have sometimes invoked scalar fields for illustrative purposes. In this chapter the idea of a classical spinor field will be introduced. We shall allow that high relative speeds may be involved; to make sure our results satisfy the Postulates of Relativity we shall only write Lorentz covariant field equations. The language of tensors and spinors makes this easy to accomplish.

A general discussion of classical field theory would require a text book in its own right. In this chapter the aim is to introduce some field equations that are close cousins of the wave equation. This will allow the basic principles of quantum field theory and particle physics to be opened up in the next chapter.

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Chapter 1

Basic Lagrangian Mechanics

The initial purpose of Lagrangian mechanics is to express the relevant equations of motion, essentially Newton's laws, in a form involving a set $q_1, q_2, \cdots, q_n$ of generalised position coordinates, and their first time-derivatives $\dot{q}_1, \dot{q}_2, \cdots, \dot{q}_n$. The n-component vector $\{\mathbf{q}\}$ can represent any physical system or process, as long as this set of numbers completely describes the state of the system (n is the number of degrees of freedom). In the most straightforward case, these can be the 3 Cartesian coordinates of a material point (a "particle"), but, say, the spherical polar set (r, θ, ϕ) is just as good. Just as $\{\mathbf{q}\}$ is the generalised coordinate vector, so is $\{\dot{\mathbf{q}}\}$ the generalised velocity, both explicit functions of time. It is assumed that simultaneous knowledge of $\{\mathbf{q}(t)\}$ and $\{\dot{\mathbf{q}}(t)\}$ completely defines the mechanical state of the system. Mathematically, this means that the complete set of $\{\mathbf{q}(t)\}$ and $\{\dot{\mathbf{q}}(t)\}$ also determines the accelerations $\{\ddot{\mathbf{q}}(t)\}$. The mathematical relations that relate accelerations with coordinates and velocities are what one calls the equations of motion.

In many cases, not all n degrees of freedom are completely free. A system may have *constraints*; for example $q_1 = \text{const.}$, $q_2 = \text{const.}, \cdots, q_r = \text{const.}$ could represent the r constraints and $q_{r+1}, \cdots, q_n$ the remaining independent coordinates. Most often the choice of generalised coordinates $\{\mathbf{q}\}$ is dictated by the nature of the constraints. For instance, if a particle is constrained to move on the surface of an expanding balloon of radius $R = a\sqrt{t}$, we might use spherical polar coordinates, scaled such that $q_1 = r/a\sqrt{t}, q_2 = \theta, q_3 = \phi$; in that case the single constraint is expressed as $q_1 = 1$ (it would look a lot more complicated if we tried to express it in Cartesians). The Lagrangian formalism is developed, partially, to enable one to deal efficiently with the sometimes complicated constraints imposed on the evolution of physical systems. Constraints are called **holonomic** if they are of the form $g(q_1, q_2, \cdots, q_n, t) = 0$. We shall shortly return to their treatment, but first, let us revise some basic starting points.

1.1 Hamilton's Principle

A very general formulation of the equations of motion of mechanical (and many other) systems is given by Hamilton's *Principle of Least Action*. It states that every mechanical system can be characterised by a certain function

$$L(q_1, q_2, \cdots, q_n; \dot{q}_1, \dot{q}_2, \cdots, \dot{q}_n; t) \equiv L(q, \dot{q}; t). \tag{1.1}$$

Theorem 1 (Hamilton's Principle)**.** *The actual motion of a system from A to B is that which makes the integral $S = \int_A^B L \, \mathrm{d}t$ a minimum.*

The function $L(q, \dot{q}; t)$ is called the Lagrangian of the given system and the integral S defined in Theorem 1 is called the **action**. Later in this course we shall have some deeper

insights into what this object, the action functional $S[\mathbf{q}(t)]$, represents and why it has to be minimal. For the time being let us take this as an axiom.

The principle of least action implies that, with a sufficient command of mathematics, in particular the calculus of variations, the solution of any mechanical problem is achieved by the following recipe:

'Minimise $S = \int_A^B L\,\mathrm{d}t$ for fixed starting and finishing (representative) points, $A = (\mathbf{q}_A, t_A)$ to $B = (\mathbf{q}_B, t_B)$, taking proper account of all the constraints.'

Remark. *There is no worldline whose action is a true maximum, that is, for which* $\delta^2 S < 0$ *or more generally for which* $S - S_0 < 0$ *for every adjacent curve.*

Proof. Here follows an intuitive proof by contradiction for the Lagrangian $L = T - V$ with T positive definite. Consider an actual worldline for which it is claimed that S is a true maximum. Now modify this worldline by adding wiggles somewhere in the middle. These wiggles are to be of very high frequency and very small amplitude so that they increase the kinetic energy T compared to that along the original worldline with only a small change in the corresponding potential energy V. The Lagrangian $L = T - V$ for the region of wiggles is larger for the new curve and so is the overall time integral S. The new worldline has greater action than the original worldline, which we claimed to have maximum action. Therefore S cannot be a true maximum for any actual worldline. □

1.2 Derivation of the Equations of Motion

First, let's examine the "standard derivation" based on d'Alembert's principle: consider a particle that is subject to the total force $\mathbf{F}$ and has momentum $\mathbf{p}$. Then if we construct a vector $(\mathbf{F} - \dot{\mathbf{p}})$, this vector will always be perpendicular to the instantaneous line of motion. In other words, the scalar product is zero:

$$\sum_i (F_i - \dot{p}_i)\delta x_i = 0. \tag{1.2}$$

That's almost trivially true for an arbitrary set of coordinate variations δx_i because Newton's second law ($\mathbf{F}^{\text{total}} = m\ddot{\mathbf{r}}$ for each particle) makes each $(F_i - \dot{p}_i) = 0$. However, we shall only be interested in sets of displacements δx_i consistent with the constraints. Constraints exert their own forces on each particle, which we call internal: see the reaction force R exerted by the wire in Fig. 1.1. By definition of the constraint, these internal forces are perpendicular to the line of motion, that is $\sum_i F_i^{\text{internal}} \delta x_i = 0$. Therefore, d'Alembert's principle states

$$\sum_i \left(F_i^{\text{internal}} - \dot{p}_i\right)\delta x_i = 0. \tag{1.3}$$

Let us try rewriting this in an arbitrary set of generalised coordinates $\{\mathbf{q}\}$ to which the Cartesians $\{\mathbf{r}\}$ could be transformed via matrices $\partial q_i/\partial x_j$. The aim is to present Eq. (1.3) as a generalised scalar product $\sum_j (\text{something})\delta q_j = 0$, so that we can say this is true for arbitrary sets of variations δq_i of the reduced number $(n - r)$ of generalised coordinate that are not subject to the constraints.

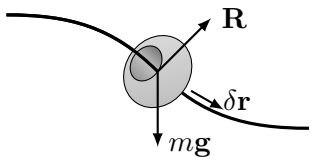

Fig. 1.1: An example of a constraint, restricting the motion of a particle (which may be subject to external forces, such as gravity) along a specific path: the bead on a wire.

The coordinate transformation in the first term, involving the external force, is easy:

$$\sum_i F_i \delta x_i = \sum_{i,j} F_i \frac{\partial x_i}{\partial q_j} \delta q_j \equiv \sum_j Q_j \delta q_j. \tag{1.4}$$

One must take great care over precisely what partial differentials mean. In the following, $\partial/\partial q_j$ means evaluating $(\partial/\partial q_j)$ with the other components $q_{i\neq j}$, all velocities $\dot{q}_i$ and time t held constant.

It is clear that $\partial x_i/\partial q_j$ should mean $(\partial x_i/\partial q_j)_{\text{all other } q,t}$; holding the $\dot{q}_i$ constant only becomes relevant when we differentiate a velocity w.r.t. q_j – a velocity component changes with $\mathbf{q}$ for fixed $\dot{\mathbf{q}}$ because the conversion factors from the $\dot{q}_j$ to the $\dot{r}_i$ change with position. Similarly, $\partial/\partial t$ means $(\partial/\partial t)_{\mathbf{q},\dot{\mathbf{q}}}$, e.g. $\partial x_i/\partial t$ refers to the change in position, for *fixed* $\mathbf{q}$ and $\dot{\mathbf{q}}$, due to the prescribed motion of the q-coordinate system.

Dealing with the second term, involving the rate of change of momentum, is a bit harder – it takes a certain amount of algebra to manipulate it into the required form. First, by definition of momentum in Cartesians:

$$\sum_i \dot{p}_i \delta x_i = \sum_{i,j} m_i \dot{v}_i \frac{\partial x_i}{\partial q_j} \delta q_j. \tag{1.5}$$

We shall need

$$v_i \equiv \dot{x}_i = \sum_j \frac{\partial x_i}{\partial q_j}\dot{q}_j + \frac{\partial x_i}{\partial t}, \quad \text{whence} \quad \frac{\partial v_i}{\partial \dot{q}_j} = \frac{\partial x_i}{\partial q_j}. \tag{1.6}$$

Now we are in a position to start work on the second term. The relevant product is

$$\dot{v}_i \frac{\partial x_i}{\partial q_j} = \frac{\mathrm{d}}{\mathrm{d}t}\left(v_i \frac{\partial x_i}{\partial q_j}\right) - v_i \frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial x_i}{\partial q_j}\right). \tag{1.7}$$

Further transforming the second term in (1.7):

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial x_i}{\partial q_j}\right) &= \frac{\partial}{\partial q_k}\left(\frac{\partial x_i}{\partial q_j}\right)\dot{q}_k + \frac{\partial}{\partial t}\left(\frac{\partial x_i}{\partial q_j}\right) \quad \text{(summed over } k\text{)} \\ &= \frac{\partial}{\partial q_j}\left[\left(\frac{\partial x_i}{\partial q_k}\right)\dot{q}_k + \frac{\partial x_i}{\partial t}\right] \\ &= \left(\frac{\partial v_i}{\partial q_j}\right)_{\text{other } q,\dot{q},t} \end{aligned} \tag{1.8}$$

Using (1.6) on the first term and (1.8) on the second term of (1.7) we finally get

$$\sum_i \dot{p}_i \delta x_i = \sum_{i,j} \left[\frac{\mathrm{d}}{\mathrm{d}t}\left(m_i v_i \frac{\partial v_i}{\partial \dot{q}_j} \right) - m_i v_i \frac{\partial v_i}{\partial q_j} \right] \delta q_j$$
$$= \sum_j \left[\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial T}{\partial \dot{q}_j} \right) - \frac{\partial T}{\partial q_j} \right] \delta q_j, \tag{1.9}$$

which is equal to $\sum_j Q_j \delta q_j$, from Eq. (1.4). Here the total kinetic energy of the system has been defined from the Cartesian representation $T = \sum_i \frac{1}{2} m_i v_i^2$. The last equation is a consequence of D'Alembert's principle. Since the components δq_j allowed by the constraints are all independent, it follows that

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial T}{\partial \dot{q}_j} \right) - \frac{\partial T}{\partial q_j} = Q_j. \tag{1.10}$$

In many systems the external forces are gradients of a scalar potential; in Cartesians:

$$F_i = -\frac{\partial V}{\partial x_i}, \quad \text{where} \quad V = V(\mathbf{x}, t), \tag{1.11}$$

(i.e. V is independent of the particle velocities), so that

$$Q_j = -\sum_i \frac{\partial V}{\partial x_i} \frac{\partial x_i}{\partial q_j} = -\frac{\partial V}{\partial q_j}. \tag{1.12}$$

Therefore, substituting this vector $\mathbf{Q}$ into the r.h.s. of Eq. (1.10) and using the fact that it does not depend on $\dot{\mathbf{q}}$, we can write

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial L}{\partial \dot{q}_j} \right) - \frac{\partial L}{\partial q_j} = 0, \tag{1.13}$$

where $L \equiv T - V$, but by construction it is a function of the generalised coordinates q, $\dot{q}$ and not the original Cartesians. We discover that this function is exactly the Lagrangian of the system, the one used in the definition of the action in Hamilton's principle. Indeed, (1.13) is the differential equation that one obtains by the calculus of variations from the condition $\delta S = 0$ for the minimum of the action.

Now let's reverse the argument. Define a function $L = T - V$. In Cartesian coordinates, an N-particle system moving in a potential $V(x_1, x_2, \cdots, x_{3N})$ has

$$p_i \equiv m_i v_i = \frac{\partial}{\partial v_i}\left(\frac{1}{2} m_i v_i^2 \right) = \frac{\partial T}{\partial v_i} \equiv \frac{\partial L}{\partial v_i}, \tag{1.14}$$

and

$$F_i = -\frac{\partial V}{\partial x_i} = \frac{\partial L}{\partial x_i}, \tag{1.15}$$

provided that V is independent of velocities, so the equations of motion $\dot{\mathbf{p}} = \mathbf{F}$ are

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial L}{\partial \dot{x}_i} \right) - \frac{\partial L}{\partial x_i} = 0. \tag{1.16}$$

Therefore the motion obeys Hamilton's principle of least action. But Hamilton's principle is a statement independent of any particular coordinate system; it is true in any coordinate

system. Therefore write down the Euler-Lagrange equations for Hamilton's principle in our new q coordinate system (in which constraints are of the kind $q_j = \text{const.}$):

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial L}{\partial \dot{q}_i}\right) - \frac{\partial L}{\partial q_i} = 0, \tag{1.17}$$

a much more memorable way to derive Lagrange's equations.

But what about the constraints? We must invent some local potentials near the actual path of the system, whose gradients are perpendicular to the actual path and just right to keep the system on the constrained trajectory, see Fig. 1.1. The important thing is that they will have no gradient along the local 'directions' of the q_is, allowed by the constraints, and will therefore not affect the dynamics for those q_is.

1.2.0.1 What is Lagrangian Mechanics Good For?

Lagrangian mechanics will do nothing that Newtonian mechanics won't do. It's just a reformulation of the same physics. In fact, it will do slightly less, because some problems (notoriously, the motion of a bicycle) have what is called non-holonomic constraints. One thing that one can say for the Lagrangian formulation is that it involves scalars (T and V) instead of vectors (forces, couples) which makes it less confusing to use in messy problems. Several examples will be treated in the lectures and, more particularly, in the examples classes. Figure 1.2 gives a few simple examples of dynamical systems with constraints. Use them to practise: in each case first write the full potential (in all cases it's gravity) and kinetic energies (don't forget the moment of inertia for the rotating cylinder), then implement the constraint (for this you need to have the appropriate choice of coordinates) and write the resulting Lagrangian, as well as the dynamical equation(s).

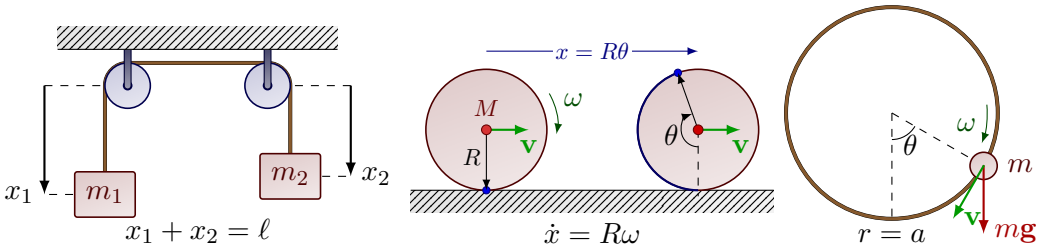

Fig. 1.2: Examples of dynamical systems with holonomic constraints (in each case their expression is in the frame). In each case the number of coordinates is reduced (for the pulley and rolling cylinder Cartesians are sufficient, the circular wire requires plane polar coordinates and rolling on the inside of a cone, spherical polar coordinates; the last case has two free generalised coordinates left).

1.2.0.2 A Few More Remarks

So far we have assumed forces depend only on position: $F_i = -\,\partial V(\mathbf{x}, t)/\partial x_i$. For *some* **velocity-dependent** forces one can still use Lagrange's equations; it's possible if you can find a $V(\mathbf{x}, \dot{\mathbf{x}}, t)$ such that

$$F_i = -\frac{\partial V(\mathbf{x}, \dot{\mathbf{x}}, t)}{\partial x_i} + \frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial V(\mathbf{x}, \dot{\mathbf{x}}, t)}{\partial \dot{x}_i}\right). \tag{1.18}$$

To derive this condition you should repeat the steps between Eqs.(1.4) and (1.13), only now allowing a contribution from V in the $\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial L}{\partial \dot{q}_i}\right)$ terms of the Euler-Lagrange equations. The hard bit is to find a V that satisfies such a condition. A bit later we shall examine the case of magnetic forces, which is a good example of such a potential.

There is also an issue of uniqueness of the Lagrangian function. Clearly the condition of zero variation $\delta[S] = 0$ can be maintained if we:

- add any constant to V;
- multiply L by any constant;
- add a total time derivative, $f = \frac{\mathrm{d}}{\mathrm{d}t}g(q, \dot{q}, t)$;

etc. Usually the convention is to take $L = T - V$, with no "additives", which then corresponds to the "classical action S".

1.3 Symmetry and Conservation Laws; Canonical Momenta

Symmetry is one of the most powerful tools used in theoretical physics. In this section we will show how symmetries of L correspond to important conservation laws. This theme will be taken further later in this course, and in subsequent solid state and particle physics courses.

When L does not depend explicitly on one of the q_i then Lagrange's equations show that the corresponding $\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial L}{\partial \dot{q}_i}\right)$ is zero, directly from Eq. (1.13). Hence we can define an object, $p_i \equiv \frac{\partial L}{\partial \dot{q}_i}$, which is conserved for such a system and q_i is called an ignorable coordinate. The object p_i is generally referred to as the *canonical momentum* corresponding to the coordinate q_i. For a particle moving in Cartesian coordinates this would be the "ordinary" momentum component: for each x_i this is just $p_i = m\dot{x}_i$. However, in generalised coordinates, the physical meaning of each component of the canonical momentum may be very different. In particular, since a generalised coordinate can have any dimensions, the dimensions of the corresponding canonical momentum need not be those of ordinary momentum.

1.3.1 Translational Invariance ↔ Conservation of Linear Momentum

Suppose L does not depend on the position of the system as a whole, i.e. we can move the position of every particle by the *same* vector ϵ without changing L. Suppose we move the whole system by δx in the x direction (in Cartesian coordinates!). Then

$$L \to L + \sum_n \frac{\partial L}{\partial x_n}\delta x. \tag{1.19}$$

(N.B. In this section and the next we sum over particles, assuming only 1-dimensional motion for simplicity: n is an index of summation over the particles. Also, V in $L = T - V$

now includes the mutual potential energies that impose e.g. the constraints that keep rigid bodies rigid.) Therefore if L does not change

$$\sum_n \frac{\partial L}{\partial x_n} = 0, \quad \text{and so, by Lagrange's equations,} \quad \sum_n \frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial L}{\partial \dot{x}_n}\right) = 0, \tag{1.20}$$

i.e. if L is independent of the position of the system $\sum \partial L/\partial \dot{x}_n$ is constant.

Now if V depends on particle positions only, then

$$\sum \frac{\partial L}{\partial \dot{x}_n} = \sum m_n \dot{x}_n \tag{1.21}$$

is just the x-component of the total momentum of the system, and we conclude

$$\text{Homogeneity of space} \implies \text{conservation of linear momentum.} \tag{1.22}$$

N.B.: This is clearly not true for velocity-dependent potentials, e.g. for charged ions moving in magnetic fields.

1.3.2 Rotational Invariance ↔ Conservation of Angular Momentum

Suppose L is independent of the orientation of the system. In particular, suppose L is invariant under rotation of the whole system about the z-axis; then, proceeding as before, we can assume a rotation by $\delta\theta$ and use cylindrical coordinates (r, θ, z) to obtain

$$\sum_n \frac{\partial L}{\partial \theta_n}\delta\theta = 0 \implies \sum_n \frac{\partial L}{\partial \theta_n} = 0 \tag{1.23}$$

$$\implies \sum_n \frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial L}{\partial \dot{\theta}_n}\right) = 0 \implies \sum_n \frac{\partial L}{\partial \dot{\theta}_n} = \text{const.} \tag{1.24}$$

Again, when V depends on particle positions only,

$$\begin{aligned}\frac{\partial L}{\partial \dot{\theta}_n} &= \frac{\partial}{\partial \dot{\theta}_n}\left(\frac{1}{2}m_n\dot{r}_n^2 + \frac{1}{2}m_n r_n^2 + \dot{\theta}_n^2 + \frac{1}{2}m_n\dot{z}_n^2\right) \\ &= m_n r_n^2 \dot{\theta}_n \qquad (1.25) \\ &= \text{ angular momentum of } n^{\text{th}} \text{ particle about } z\text{-axis} \qquad (1.26)\end{aligned}$$

Thus the total angular momentum about the z axis is conserved.

$$\text{Isotropy of space} \implies \text{conservation of angular momentum.} \tag{1.27}$$

1.3.3 Time Invariance ↔ Conservation of Energy

This is a bit more complicated and it also gives us a chance to explore a very useful mathematical result called Euler's homogeneous function theorem. If L does not depend explicitly on time, i.e.

$$L = L(q_i\dot{q}_i) \implies \frac{\partial L}{\partial t} = 0, \tag{1.28}$$

then the total time derivative of the Lagrangian is

$$\frac{\mathrm{d}L}{\mathrm{d}t} = \sum_i \frac{\partial L}{\partial q_i}\dot{q}_i + \sum_i \frac{\partial L}{\partial \dot{q}_n}\ddot{q}_n \tag{1.29}$$

$$= \sum_i \frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial L}{\partial q_i}\right)\dot{q}_i + \sum_i \frac{\partial L}{\partial \dot{q}_i}\ddot{q}_n \quad \text{(using the E-L equation)}$$

$$= \sum_i \frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial L}{\partial \dot{q}_i}\dot{q}_i\right) \quad \text{(assembling the total derivative from both terms)}, \tag{1.30}$$

or, combining the total time derivatives from l.h.s. and r.h.s. into one expression, we have

$$0 = \frac{\mathrm{d}}{\mathrm{d}t}H, \quad \text{where} \quad H = \sum_i \frac{\partial L}{\partial \dot{q}_i}\dot{q}_i - L = \text{a constant, } E \tag{1.31}$$

We shall now identify the new function H, the **Hamiltonian**, as the total energy of the system. Assume the generalised kinetic energy, T, is given by:

$$T = \sum_{i,j} \frac{1}{2} c_{ij}\dot{q}_i\dot{q}_j, \tag{1.32}$$

where we can generically choose $c_{ij} = c_{ji}$ (by symmetry of dummy indices of summation). The coefficients c_{ij} might be functions of $q_1, \cdots, q_n$ but not $\dot{q}_1, \cdots, \dot{q}_n$ or time. This quadratic form is also called a homogeneous second-order polynomial function of $\dot{\mathbf{q}}$. Assume also that the potential energy, V, is given by:

$$V = V(q_1, \cdots, q_n), \tag{1.33}$$

(velocity-independent) and $L = T - V$ as usual (with no explicit time-dependence as we agreed). Then:

$$\sum_i \frac{\partial L}{\partial \dot{q}_i}\dot{q}_i = \sum_i \dot{q}_i \frac{\partial}{\partial \dot{q}_i}\left(\sum_{j,k} \frac{1}{2} c_{jk}\dot{q}_j\dot{q}_k\right) \quad \text{since} \quad \frac{\partial V}{\partial \dot{q}_i} = 0 \tag{1.34}$$

$$= \sum_i \dot{q}_i \left(\sum_{j,k} \left[\frac{1}{2} c_{jk}\delta_{jk}\dot{q}_k + \frac{1}{2} c_{jk}\dot{q}_j\delta_{ik}\right]\right) \quad \text{since} \quad \frac{\partial \dot{q}_j}{\partial \dot{q}_i} = \delta_{ij}$$

$$= \sum_i \dot{q}_i \left(\sum_k \frac{1}{2} c_{ik}\dot{q}_k + \sum_j \frac{1}{2} c_{ji}\dot{q}_j\right)$$

$$= \sum_i \dot{q}_i \left(\sum_j c_{ij}\dot{q}_j\right) \quad \text{renaming the dummy index } k \to j$$

$$= \sum_{i,j} c_{ij}\dot{q}_i\dot{q}_j$$

$$= 2T. \tag{1.35}$$

In effect, what we have just proven is that for any homogeneous quadratic function $T = T(q_i)$, the following property holds:

$$\sum_i q_i \frac{\partial T}{\partial q_i} = 2T \tag{1.36}$$

(an aspect of Euler's more general theorem; guess how this would change for linear, or cubic functions). Returning to our Hamiltonian, we have $H = 2T - L = 2T - (T - V) = T + V \equiv$ total energy $= E$, a constant from Eq. (1.31).

Chapter 2

Hamilton's Equations of Motion

We have already defined the i^{th} component of generalised (canonical) momentum as

$$p_i \equiv \left(\frac{\partial L}{\partial \dot{q}_i}\right)_{\text{other } \dot{q},\mathbf{q},t} \tag{2.1}$$

In Cartesians and for $V = V(\mathbf{r})$, $p_i = m_i v_i$.

Now try to re-write the equations of motion in terms of $\mathbf{q}$ and $\mathbf{p}$ instead of $\mathbf{q}$ and $\dot{\mathbf{q}}$. This operation is fully analogous to what is called the Legendre transformation in thermodynamics, when we change from one potential depending on a given variable to another, depending on its conjugate (like $T\,\mathrm{d}S \to -S\,\mathrm{d}T$ or $-p\,\mathrm{d}V \to V\,\mathrm{d}p$).

The Euler-Lagrange equations say

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial L}{\partial \dot{q}_i}\right) \equiv \dot{p}_i = \left(\frac{\partial L}{\partial q_i}\right)_{\text{other } q,\dot{\mathbf{q}},t}, \tag{2.2}$$

but that's not quite what we want, for it refers to $L(\mathbf{q}, \dot{\mathbf{q}}, t)$, not $L(\mathbf{q}, \mathbf{p}, t)$. We proceed thus:

$$\begin{aligned} \delta L &= \frac{\partial L}{\partial t}\delta t + \sum_i \frac{\partial L}{\partial q_i}\delta q_i + \sum_i \frac{\partial L}{\partial \dot{q}_i}\delta \dot{q}_i \\ &= \frac{\partial L}{\partial t}\delta t + \sum_i \dot{p}_i \delta q_i + \sum_i p_i \delta \dot{q}_i. \end{aligned} \tag{2.3}$$

Hence

$$\delta\left(L - \sum_i p_i \dot{q}_i\right) = \frac{\partial L}{\partial t}\delta t + \sum_i \dot{p}_i \delta q_i - \sum_i \dot{q}_i \delta p_i. \tag{2.4}$$

This last equation suggests that the expression in brackets on the l.h.s. is a function of (t, q, p). It is clear that every pair of a generalised velocity $\dot{q}_i$ and its canonical momentum p_i have the same status as conjugate variables in thermodynamics. (Of course, historically, people developed the underlying maths behind Lagrangian and Hamiltonian dynamics first; the physical concepts of thermodynamics were then easy to formalise.)

Defining the Hamiltonian as in Eq. (1.31):

$$H \equiv \left(\sum_i p_i \dot{q}_i - L\right)\Bigg|_{\dot{q}_i = \dot{q}_i(\mathbf{q},\mathbf{p},t)}, \tag{2.5}$$

then (2.4) implies

$$\dot{p}_i = -\left(\frac{\partial H}{\partial q_i}\right)_{\text{other } q,\mathbf{p},t} \qquad \dot{q}_i = \left(\frac{\partial H}{\partial p_i}\right)_{\text{other } p,\mathbf{q},t}, \tag{2.6}$$

which are **Hamilton's equations of motion**. Notice the importance of completing the transformation in Eq. (2.5) and writing H as a function of $\mathbf{q}, \mathbf{p}, t$ only. None of the $\dot{q}_i$

should appear explicitly; rather, they should be replaced by inverting Eq.(2.1) that defines p_i.

We have already shown that, provided L does not depend explicitly on time, T has the form (1.32) and V does not depend on velocities, then $H = T + V$, the total energy, and it is a constant of the motion. This does not imply that the right-hand sides of Hamilton's equations are zero! They are determined by the functional form of the dependence of H on the p_i and q_i.

Note also that p_i and q_i are now on an equal footing. In Hamilton's equations q_i can be anything, not necessarily a position coordinate. For example we could interchange the physical meaning of what we regard as p_i with q_i, and q_i with $-p_i$, and Hamilton's equations would still work.

Advantages of the Hamiltonian formulation over the Lagrangian formulation include:

- The Lagrangian formulation leads to N second order differential equations while the Hamiltonian formulation leads to $2N$ first order differential equations, which may be easier to solve.
- The q_i in the Lagrangian formulation must be position co-ordinates, whereas in the Hamiltonian formulation the q_i and p_i are on an equal footing and the q_i need not be position co-ordinates. This also means that canonical transformations with mixed momenta and postion can be used to greatly simplify Hamilton's equations.
- The Hamiltonian formulation can lead to easily identifiable constants of motion (for example, if H is independent of t then energy is conserved). The presence of a conserved quantity immediately simplifies Hamilton's equations, whereas no immediate simplification would occur in the Lagrangian formulation.
- There is a simple relationship between the (classical) Hamiltonian formulation and quantum mechanics.

2.1 Liouville's theorem

Phase space is defined as the space spanned by the canonical coordinates and conjugate momenta, e.g. (x, y, z, p_x, p_y, p_z) for a single particle (a 6D space) and $\{q_1, q_2, \cdots, q_n, p_1, p_2, \cdots, p_n\}$ for a system of n particles. This defines phase space to be a $6n$-dimensional space. A single point in phase space represents the state of the whole system, i.e. the positions and velocities of all its particles. It is called a **representative point**. If there are constraints acting on the system, the representative points are confined to some lower dimensional subspace. The representative points move with velocities $\mathbf{v}$ where:

$$\mathbf{v} = \{\dot{q}_1, \dot{q}_2, \cdots, \dot{q}_n, \dot{p}_1, \dot{p}_2, \cdots, \dot{p}_n\} = \left\{\frac{\partial H}{\partial p_1}, \frac{\partial H}{\partial p_2}, \cdots, \frac{\partial H}{\partial p_n}, -\frac{\partial H}{\partial q_1}, -\frac{\partial H}{\partial q_2}, \cdots, -\frac{\partial H}{\partial q_n}\right\}. \tag{2.7}$$

Liouville's theorem is a very powerful result concerning the evolution in time of ensembles of systems. We can regard the initial state of the ensemble of systems as corresponding to

a distribution or density of representative points in phase space. Then Liouville's theorem states that:

Theorem 2 (Liouville's theorem)**.** *The density in phase space evolves as an incompressible fluid.*

Proof. The proof is a simple application of Hamilton's equations and the n-dimensional divergence theorem. The n-dimensional divergence theorem states that for an n-dimensional vector function of n variables $\mathbf{V}(x_1, \cdots, x_n)$:

$$\int_{\mathcal{V}} \sum_i \frac{\partial V_i}{\partial x_i} \, \mathrm{d}\tau = \int_{\mathcal{S}} \sum_i V_i \, \mathrm{d}S_i \,, \tag{2.8}$$

where $\mathrm{d}\tau$ is an n-dimensional volume element and $\mathrm{d}\mathbf{S}$ is an $(n-1)$-dimensional element of surface area. This theorem and its proof are the obvious generalisation the divergence theorem (the Gauss theorem) in 3D:

$$\int_{\mathcal{V}} \boldsymbol{\nabla} \cdot \mathbf{V} \, \mathrm{d}\tau = \int_{\mathcal{S}} \mathbf{V} \cdot \mathrm{d}\mathbf{S} \,. \tag{2.9}$$

To prove Liouville's theorem, suppose that the representative points are initially confined to some (n-dimensional) volume $\mathcal{V}$ with surface $\mathcal{S}$. The points move with velocity $\mathbf{v}$ given by Eq. (2.7). Therefore, at the surface, the volume occupied by the points is changing at a rate $\mathrm{d}V = \mathbf{v} \cdot \mathrm{d}\mathbf{S}$. Hence:

$$\begin{aligned} \Delta V &= \int_{\mathcal{S}} \mathbf{v} \cdot \mathrm{d}\mathbf{S} \\ &= \int_{\mathcal{V}} \boldsymbol{\nabla} \cdot \mathbf{v} \, \mathrm{d}\tau \,, \end{aligned} \tag{2.10}$$

by (2.9). However,

$$\begin{aligned} \boldsymbol{\nabla} \cdot \mathbf{v} &= \sum_i \frac{\partial}{\partial q_i} \dot{q}_i + \frac{\partial}{\partial p_i} \dot{p}_i \\ &= \sum_i \frac{\partial^2 H}{\partial q_i \partial p_i} - \frac{\partial^2 H}{\partial p_i \partial q_i} = 0. \end{aligned} \tag{2.11}$$

So the volume occupied by the ensemble's representative points does not change. □

2.2 Poisson Brackets and the Analogy with Quantum Commutators

Suppose $f = f(q_i, p_i, t)$, i.e. f is a function of the dynamical variables $\mathbf{p}$ and $\mathbf{q}$. Then

$$\frac{\mathrm{d}f}{\mathrm{d}t} = \frac{\partial f}{\partial q_i} \dot{q}_i + \frac{\partial f}{\partial p_i} \dot{p}_i + \frac{\partial f}{\partial t} \tag{2.12}$$

$$= \frac{\partial f}{\partial q_i} \frac{\partial H}{\partial p_i} - \frac{\partial f}{\partial p_i} \frac{\partial H}{\partial q_i} + \frac{\partial f}{\partial t}, \tag{2.13}$$

which we can rewrite for notational convenience as

$$\frac{\mathrm{d}f}{\mathrm{d}t} = \{f, H\} + \frac{\partial f}{\partial t}, \tag{2.14}$$

where

$$\{f, g\} \equiv \frac{\partial f}{\partial q_i}\frac{\partial g}{\partial p_i} - \frac{\partial f}{\partial p_i}\frac{\partial g}{\partial q_i}, \tag{2.15}$$

is called the *Poisson Bracket* of the functions f and g and was first introduced into mechanics by Simon Poisson in 1809 (Note the use of summation convention in Eq. (2.15)).

Eq. (2.14) is remarkably similar to the Ehrenfest theorem in Quantum Mechanics

$$\frac{\mathrm{d}}{\mathrm{d}t}\left\langle \hat{O} \right\rangle = \frac{1}{i\hbar}\left\langle \left[\hat{O}, \hat{H}\right] \right\rangle + \left\langle \frac{\partial \hat{O}}{\partial t} \right\rangle, \tag{2.16}$$

for the variation of expectation values of (Hermitian) operators $\hat{O}$, where $\hat{H}$ is of course the quantum mechanical Hamiltonian operator and $\left[\hat{O}, \hat{H}\right]$ represents the commutator $\hat{O}\hat{H} - \hat{H}\hat{O}$.

It is easy to check that $\{f, g\}$ has many of the properties of the commutator:

$$\{f, g\} = -\{g, f\}, \quad \{f, f\} = 0 \quad \text{etc.} \tag{2.17}$$

Also, if in Eq. (2.12) $\partial f/\partial t = 0$ (no explicit t dependence) and $\{f, H\} = 0$ then $\mathrm{d}f/\mathrm{d}t = 0$, i.e. f is a constant of the motion.

This suggests we can relate classical and quantum mechanics by formulating classical mechanics in terms of Poisson Brackets and then associating these with the corresponding Quantum Mechanical commutator

$$\begin{gathered} \{A, B\} \leftrightarrow \frac{1}{i\hbar}\left[\hat{A}, \hat{B}\right] \\ \text{classical} \leftrightarrow \text{quantum} \\ H \leftrightarrow \hat{H}. \end{gathered} \tag{2.18}$$

Classically

$$\{q, p\} = \frac{\partial q}{\partial p}\frac{\partial p}{\partial p} - \frac{\partial q}{\partial p}\frac{\partial p}{\partial q} = 1. \tag{2.19}$$

Quantum Mechanically,

$$\left[q, -i\hbar\frac{\partial}{\partial q}\right]\Psi = -qi\hbar\frac{\partial}{\partial q}\Psi + i\hbar\frac{\partial}{\partial q}(q\Psi) = i\hbar\Psi, \tag{2.20}$$

i.e.

$$\frac{1}{i\hbar}\left[q, -i\hbar\frac{\partial}{\partial q}\right] = 1 = \{q, p\}. \tag{2.21}$$

Therefore we confirm the identification of $-i\hbar\,\partial/\partial q$ with the canonical **momentum operator** $\hat{p}$ corresponding to q.

2.2.1 Quantum Variational Principle

In QM we associate a wave vector $\mathbf{k} = \mathbf{p}/\hbar$ with a particle of momentum p (de Broglie relation), and frequency $\omega = H/\hbar$ with its total energy $E = H$ (Einstein relation). Thus we can write Hamilton's principle for the classical motion of the particle as

$$\frac{1}{\hbar}\int L\,\mathrm{d}t = \int\left(\frac{1}{\hbar}\mathbf{p}\cdot\dot{\mathbf{q}} - \frac{H}{\hbar}\right)\mathrm{d}t = \int(\mathbf{k}\cdot\mathrm{d}\mathbf{q} - \omega\,\mathrm{d}t) = \text{stationary}, \tag{2.22}$$

i.e. the wave-mechanical phase shall be stationary (because multiplication by a constant factor does not alter the condition for the minimum of S). This is the condition for constructive interference of waves; what the Hamilton principle really says is that the particle goes where the relevant de Broglie waves reinforce. If we move a little away from the classical path, the waves do not reinforce so much and the particle is less likely to be found there. If we imagine taking the limit $\hbar \to 0$, the wavefunction falls off so rapidly away from the classical path that the particle will *never* deviate from it.

We see that classical mechanics is the "geometrical optics" limit of QM: the "rays" correspond to the classical paths and quantum effects (like diffraction) are due the finite frequency and wave number of waves of given energy and momentum, i.e the finite value of $\hbar$.

Conversely, if we have a classical theory for a physical system, which works for macroscopic systems of that kind, we can get a wave-mechanical description that reduces to this classical theory as $\hbar \to 0$ by making the Hamiltonian operator $\hat{H}$ the same function of $-i\hbar\,\partial/\partial q_i$ and q_i as the classical Hamiltonian H is of p_i and q_i.

N.B.: This is not necessarily the only or the correct QM description! There may be other bits of physics (terms in H) which vanish as $\hbar \to 0$ but are important, e.g., the electron spin.

2.2.2 Canonical Transformations

Another advantage of the Hamiltonian formulation of dynamics is that we have considerable freedom to redefine the generalised coordinates and momenta, which can be useful for solving the equations of motion. For example, as we already saw, we can redefine p_i as q_i and q_i as $-p_i$. This is an example of a much more general change of variables known as a *canonical transformation*. This is a transformation of the form

$$Q_j = Q_j(\{q_i\},\{p_i\}), \quad P_j = P_j(\{q_i\},\{p_i\}), \tag{2.23}$$

that preserves the form of Hamilton's equations of motion:

$$\dot{P}_j = -\left(\frac{\partial H}{\partial Q_j}\right)_{\text{other } Q,\mathbf{P},t}, \quad \dot{Q}_j = -\left(\frac{\partial H}{\partial P_j}\right)_{\text{other } P,\mathbf{Q},t}. \tag{2.24}$$

The condition for a transformation to be canonical is very simple: the transformed variables have to satisfy the canonical Poisson bracket relations

$$\{Q_j, P_j\} = 1, \quad \{Q_j, Q_k\} = \{P_j, P_k\} = \{Q_j, P_k\} = 0 \quad \text{for} \quad j \neq k, \tag{2.25}$$

with respect to the original generalised coordinates and momenta. We prove this for a single coordinate and momentum; the generalization to many variables is straightforward. For any function $Q(q,p)$, not explicitly time-dependent, we have

$$\dot{Q} = \{Q, H\} = \frac{\partial Q}{\partial q}\frac{\partial H}{\partial p} - \frac{\partial Q}{\partial p}\frac{\partial H}{\partial q}. \tag{2.26}$$

Expressing H in terms of Q and some other function $P(q,p)$,

$$\frac{\partial H}{\partial p} = \frac{\partial H}{\partial Q}\frac{\partial Q}{\partial p} + \frac{\partial H}{\partial P} + \frac{\partial P}{\partial p} \tag{2.27}$$

$$\frac{\partial H}{\partial q} = \frac{\partial H}{\partial Q}\frac{\partial Q}{\partial q} + \frac{\partial H}{\partial P} + \frac{\partial P}{\partial q}. \tag{2.28}$$

Inserting these in Eq. (2.26) and rearranging terms,

$$\begin{aligned}\dot{Q} &= \frac{\partial H}{\partial P}\left(\frac{\partial Q}{\partial q}\frac{\partial P}{\partial p} - \frac{\partial Q}{\partial p}\frac{\partial P}{\partial q}\right) \\ &= \frac{\partial H}{\partial P}\{Q, P\}.\end{aligned} \tag{2.29}$$

Similarly for P we find

$$\begin{aligned}\dot{P} &= \frac{\partial H}{\partial Q}\left(\frac{\partial P}{\partial q}\frac{\partial Q}{\partial p} - \frac{\partial P}{\partial p}\frac{\partial Q}{\partial q}\right) \\ &= -\frac{\partial H}{\partial Q}\{Q, P\}.\end{aligned} \tag{2.30}$$

Hence the necessary and sufficient condition to preserve Hamilton's equations is $\{Q, P\} = 1$.

2.3 Lagrangian Dynamics of a Charged Particle

The Lorentz force is an example of a velocity dependent force. Another example is the 'fictitious' Coriolis force found in rotating (non-inertial) frames. A deeper treatment of these forces leads to special relativity in the case of electromagnetism and general relativity in the case of inertial forces.

In this section we examine how the Lorentz force and basic electromagnetism can be incorporated into the Lagrangian formalism without explicit mention of special relativity. In the following sections we sketch the much more powerful ideas involved in the relativistic approach.

The derivation of Lagrange's equations of motion is valid provided the external forces satisfy

$$F_i = -\frac{\partial V}{\partial x_i} + \frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial V}{\partial \dot{x}_i}\right). \tag{2.31}$$

The second term (with the derivative w.r.t. velocity) is *not* usually present for conventional (i.e. potential, $\mathbf{F} = -\boldsymbol{\nabla} V$) forces. For the Lorentz force problem, a particle of charge e in fields $\mathbf{E}$ and $\mathbf{B}$ experiences a velocity dependent force $\mathbf{F}$,

$$\mathbf{F} = e(\mathbf{E} + \mathbf{v} \times \mathbf{B}), \tag{2.32}$$

and we can in fact take

$$V = e(\phi - \mathbf{v}\cdot\mathbf{A}), \tag{2.33}$$

where $\mathbf{A}$ is the magnetic vector potential such that $\mathbf{B} = \boldsymbol{\nabla}\times\mathbf{A}$ and $\mathbf{E} = -\boldsymbol{\nabla}\phi - \partial\mathbf{A}/\partial t$.

The potential (2.33), when plugged into (2.31), gives the correct expression for the force (2.32). To verify this, we need to perform a calculation:

$$F_i = e(\mathbf{E} + \mathbf{v}\times\mathbf{B})_i \stackrel{?}{=} -\frac{\partial V}{\partial x_i} + \frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial V}{\partial \dot{x}_i}\right). \tag{2.34}$$

We will need the result of vector analysis

$$[\mathbf{v}\times(\boldsymbol{\nabla}\times\mathbf{A})]_i = v_j\frac{\partial A_j}{\partial x_i} - v_j\frac{\partial A_i}{\partial x_j}, \tag{2.35}$$

which follows from

$$\begin{aligned}
[\mathbf{v}\times(\boldsymbol{\nabla}\times\mathbf{A})]_i &= \epsilon_{ijk}v_j(\boldsymbol{\nabla}\times\mathbf{A})_k && (2.36)\\
&= \epsilon_{ijk}v_j\epsilon_{kpq}\frac{\partial A_q}{\partial x_p} && (2.37)\\
\epsilon_{ijk}\epsilon_{pqk} \equiv (\delta_{ip}\delta_{jq} - \delta_{iq}\delta_{jp}) \quad\Longrightarrow\quad &= (\delta_{ip}\delta_{jq} - \delta_{iq}\delta_{jp})v_j\frac{\partial A_q}{\partial x_p}\\
&= v_j\frac{\partial A_j}{\partial x_i} - v_j\frac{\partial A_i}{\partial x_j}. && (2.38)
\end{aligned}$$

The rest is a simple manipulation

$$\begin{aligned}
F_i &= -\frac{\partial V}{\partial x_i} + \frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial V}{\partial v_i}\right) && (2.39)\\
&= -\frac{\partial}{\partial x_i}e(\phi - v_jA_j) + \frac{\mathrm{d}}{\mathrm{d}t}(-eA_i)\\
&= -e\frac{\partial\phi}{\partial x_i} + ev_j\frac{\partial A_j}{\partial x_i} - e\frac{\partial A_i}{\partial x_j}v_j - e\frac{\partial A_i}{\partial t}\\
&= e(\mathbf{E} + [\mathbf{v}\times(\boldsymbol{\nabla}\times\mathbf{A})])_i. && (2.40)
\end{aligned}$$

Having satisfied our sense of caution to some extent, we can now write the Lagrangian, as usual,

$$L = T - V = \frac{1}{2}mv^2 - e(\phi - \mathbf{v}\cdot\mathbf{A}). \tag{2.41}$$

The components of the canonical momentum $\mathbf{p}$ are obtained by the familiar

$$p_i = \frac{\partial L}{\partial \dot{x}_i} = \frac{\partial L}{\partial v_i} = mv_i + eA_i, \tag{2.42}$$

or, for a charged particle in an electromagnetic field,

$$\text{canonical momentum} = \text{mechanical momentum} + e\mathbf{A}. \tag{2.43}$$

Knowing p_i we can write down the Hamiltonian H, formally following our previous definitions,

$$\begin{aligned} H &= \mathbf{p}\cdot\dot{\mathbf{q}} - L \qquad (2.44)\\ &= (m\mathbf{v} + e\mathbf{A})\cdot\mathbf{v} - \frac{1}{2}mv^2 + e(phi - \mathbf{v}\cdot\mathbf{A})\\ &= \frac{1}{2}mv^2 + e\phi \quad \text{(total energy)}\\ &= \frac{1}{2m}(\mathbf{p} - e\mathbf{A})^2 + e\phi, \qquad (2.45) \end{aligned}$$

where $\mathbf{p}$ is the canonical momentum (2.42).

Suppose we reverse the argument and formally start from the Lagrangian (2.41), looking for the equations of motion by minimisation of the corresponding action:

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial L}{\partial \mathbf{v}}\right) = \frac{\partial L}{\partial \mathbf{x}} \equiv \boldsymbol{\nabla} L = e\boldsymbol{\nabla}(\mathbf{v}\cdot\mathbf{A}) - e\boldsymbol{\nabla}\phi. \qquad (2.46)$$

Another useful formula from vector analysis says:

$$\boldsymbol{\nabla}(\mathbf{a}\cdot\mathbf{b}) = (\mathbf{a}\cdot\boldsymbol{\nabla})\mathbf{b} + (\mathbf{b}\cdot\boldsymbol{\nabla})\mathbf{a} + \mathbf{a}\times(\boldsymbol{\nabla}\times\mathbf{b}) + \mathbf{b}\times(\boldsymbol{\nabla}\times\mathbf{a}), \qquad (2.47)$$

for any two vectors $\mathbf{a}$ and $\mathbf{b}$. Remembering that $\boldsymbol{\nabla} L$ in (2.46) is evaluated at constant $\mathbf{v}$, we find for its r.h.s.

$$\boldsymbol{\nabla} L = e(\mathbf{v}\cdot\boldsymbol{\nabla})\mathbf{A} + e[\mathbf{v}\times(\boldsymbol{\nabla}\times\mathbf{A})] - e\boldsymbol{\nabla}\phi. \qquad (2.48)$$

The l.h.s. of (2.46) is the total time-derivative of the canonical momentum $\mathbf{p} = m\mathbf{v} + e\mathbf{A}$. The total time-derivative of $\mathbf{A}$, which may be a function of time and position, is given by

$$\frac{\mathrm{d}\mathbf{A}}{\mathrm{d}t} + \frac{\partial \mathbf{A}}{\partial t} + (\mathbf{v}\cdot\boldsymbol{\nabla})\mathbf{A}. \qquad (2.49)$$

Substituting this and (2.48) into (2.46) we find that the awkward $(\mathbf{v}\cdot\boldsymbol{\nabla})$ term cancels and the equation of motion becomes

$$\frac{\mathrm{d}(m\mathbf{v})}{\mathrm{d}t} = -e\frac{\partial \mathbf{A}}{\partial t} - e\boldsymbol{\nabla}\phi + e[\mathbf{v}\times(\boldsymbol{\nabla}\times\mathbf{A})]. \qquad (2.50)$$

The force on the r.h.s. is thus made up of two parts. The first (the first two terms) does not depend on the particle velocity; the second part is proportional to $|\mathbf{v}|$ and is perpendicular to it. The first force, per unit of particle charge e, is *defined* as the **electric field**,

$$\mathbf{E} = -\boldsymbol{\nabla}\phi - \frac{\partial \mathbf{A}}{\partial t}, \qquad (2.51)$$

and the force proportional to the velocity, per unit charge, is *defined* as the **magnetic flux density**

$$\mathbf{B} = \boldsymbol{\nabla}\times\mathbf{A}, \qquad (2.52)$$

which returns the familiar expression for the full Lorentz force (2.32).

2.3.1 Gauge Invariance

The equation of motion of a physical particle is determined by the physically observable fields **E** and **B**. How unique are the potentials ϕ and **A** which determine these fields and contribute to the Lagrangian function? It turns out that they are not unique at all ...

If we add the gradient of an arbitrary scalar function $f(\mathbf{x}, t)$ to the vector potential **A**, i.e.

$$A_i' = A_i + \frac{\partial f}{\partial x_i}, \tag{2.53}$$

the magnetic flux density **B** will not change, because $\boldsymbol{\nabla} \times \boldsymbol{\nabla} f \equiv 0$. To have the electric field unchanged as well, we must simultaneously subtract the time-derivative of f from the scalar potential:

$$\phi' = \phi - \frac{\partial f}{\partial t}. \tag{2.54}$$

The invariance of all electromagnetic processes with respect to the above transformation of the potentials by an arbitrary function f is called **gauge invariance**. As always, the discovery of an additional symmetry is an indication of much deeper underlying physics and you will meet gauge invariance, and its consequences, many times in the future.

But how are we to deal with such non-uniqueness of the electromagnetic potentials and, accordingly, the Lagrangian? Because an arbitrary scalar function is governing the invariance transformation, one is free to choose *any* additional condition, an equation relating the potentials ϕ and **A** – but only one such condition. For instance, we may choose to formulate electrodynamics with no scalar electric potential, $\phi = 0$. However we cannot have $\mathbf{B} = \mathbf{0}$, since this represents three conditions for its components, instead of the allowed one. We can at most choose $\mathbf{n} \cdot \mathbf{A} = 0$ for some constant vector **n**. Vector potentials satisfying such a condition are said to be in an *axial gauge*, with gauge vector **n**.

Alternatively , since one can add an arbitrary gradient to **A**, we could enforce the condition $\boldsymbol{\nabla} \cdot \mathbf{A} = 0$. Potentials satisfying this condition are said to be in the *Coulomb gauge*. Such a gauge leads to a convenient form of wave equation for **A**, used in the theory of electromagnetic waves.

In relativistic dynamics, a commonly used condition is

$$\frac{\partial \phi}{\partial t} + \boldsymbol{\nabla} \cdot \mathbf{A} = 0, \tag{2.55}$$

which defines the *Lorenz gauge*. Notice that in this gauge there remains a residual ambiguity: we can still vary the electromagnetic potentials using any function f that satisfies the wave equation

$$\frac{\partial^2 f}{\partial t^2} - \nabla^2 f = 0. \tag{2.56}$$

2.4 Relativistic Particle Dynamics

The 4-index or **covariant notation** is widely used in theoretical physics; this subsection contains a brief (and not very rigorous) introduction. Consider:

$$x^\mu : (x^0, x^1, x^2, x^3) = (ct, x, y, z) \quad \text{a } \textbf{contravariant} \text{ 4-vector and} \tag{2.57}$$

$$x_\mu : (x_0, x_1, x_2, x_3) = (ct, -x, -y, -z) \quad \text{a } \textbf{covariant} \text{ 4-vector.} \tag{2.58}$$

Only (implicit) summations involving one raised and one lowered suffix are allowed, thus:

$$x^\mu x_\mu = c^2t^2 - r^2, \tag{2.59}$$

is valid (and is of course Lorentz invariant), but neither $x^\mu x^\mu$ nor $x_\mu x_\mu$ is allowed.

If $\phi = \phi(x^\mu)$ then $\mathrm{d}\phi = \frac{\partial\phi}{\partial x^\mu}\,\mathrm{d}x^\mu$ is invariant, hence:

$$\frac{\partial\phi}{\partial x^\mu} \quad \text{is a covariant 4-vector and} \tag{2.60}$$

$$\frac{\partial}{\partial x^\mu} \quad \text{is a covariant operator.} \tag{2.61}$$

The operator $\frac{\partial}{\partial x^\mu}$ is often simply written as ∂_μ. Similarly the contravariant operator $\frac{\partial}{\partial x_\mu} = \partial^\mu$. The "metric tensor":

$$g_{\mu\nu} = g^{\mu\nu} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} \tag{2.62}$$

can be used to raise or lower indices, for example:

$$x_\mu = g_{\mu\nu}x^\nu, \quad \text{etc.} \tag{2.63}$$

Finally we remark that in General Relativity $g^{\mu\nu}$ becomes a function of the mass distribution.

2.4.1 Relativistic Lagrangians

To derive the Lagrangian for a relativistic particle, we will begin from the equation of motion

$$\frac{\mathrm{d}\mathbf{p}}{\mathrm{d}t} = -\boldsymbol{\nabla}V, \tag{2.64}$$

but of course the relativistic momentum is more complicated and the simple recipe "$L = T - V$" can be readily checked *not* to work.

Two possible routes to the relativistic Lagrangian are instructive. First let us try guessing that $\gamma(v)m\mathbf{v}$ is the canonical momentum, which then requires

$$\frac{\partial L}{\partial \mathbf{v}} = \gamma(v)m\mathbf{v}. \tag{2.65}$$

Integrating this with respect to v (using explicitly that $\gamma = \left[1 - v^2/c^2\right]^{-1/2}$) then gives

$$L(\mathbf{r}, \mathbf{v}) = -\frac{1}{\gamma(v)} mc^2 - f(\mathbf{r}). \tag{2.66}$$

The 'constant of integration' $f(\mathbf{r})$ is readily determined as $V(\mathbf{r})$ by requiring that the Euler-Lagrange equations get the r.h.s. of the equation of motion correctly. You can recover the familiar non-relativistic limit by expanding in powers of v/c, and discarding the constant $-mc^2$.

The second method is more elegant but specialised to relativistic principles: let us analyse the motion in a frame of reference where it is non-relativistic, and then rewrite the analysis in a manner which is evidently frame-independent. This should then apply even when the motion appears highly relativistic. We saw that one can write the Lagrangian Action as

$$S = \int L \, \mathrm{d}t = \int (\mathbf{p} \cdot \mathrm{d}\mathbf{r} - H \, \mathrm{d}t). \tag{2.67}$$

Now $(H, c, \mathbf{p}) = p^\mu$, the (contravariant) 4-momentum, and hence we can write this in terms of four-vectors as

$$S = -\int p^\mu \, \mathrm{d}x_\mu = -\int p_\mu \, \mathrm{d}x^\mu \, . \tag{2.68}$$

Now $p_\mu \, \mathrm{d}x^\mu$ is frame-independent, and in the comoving frame of a free particle it evaluates to $mc^2 \, \mathrm{d}\tau$, where τ is the proper time. All observers thus agree on this form for the action, and for a free particle it obviously matches $mc^2\gamma(v) \, \mathrm{d}t$ which we got before.

The result is that for a free relativistic particle, the trajectory from one point in space-time (=event) to another fixed event is that which maximises the elapsed proper time. Because the equations of motion are only obeyed *after* maximising, it should be clarified that the proper time is to be evaluated on the basis of $\mathrm{d}\tau = \mathrm{d}t \, /\gamma(v)$ – that is the form for which we showed that the Euler-Lagrange equations gave the right results.

2.4.2 Relativistic Particle in Electromagnetic Field

To cope with EM interactions relativistically, we generalise the non-relativistic contribution to the action, $-\int V \, \mathrm{d}t$, to a four-vector EM potential interaction contribution, $-e \int (\phi \, \mathrm{d}t - \mathbf{A} \cdot \mathrm{d}\mathbf{r}) = -e \int A_\mu \, \mathrm{d}x^\mu$, where the scalar electric potential ϕ has been absorbed as the timelike component $\phi/c = A_t$ of the EM 4-potential and a factor of charge e has been introduced. Then the action becomes

$$S = -\int mc^2 \, \mathrm{d}\tau - \int eA_\mu \, \mathrm{d}x^\mu \, . \tag{2.69}$$

$$\text{free particle} + \text{interaction with field}. \tag{2.70}$$

Now we have to be very careful to distinguish between the mechanical momentum $\mathbf{p}^{\text{mechanical}}$ $= \gamma m \mathbf{v}$ and the canonical momentum $\mathbf{p}^{\text{canonical}} = \partial L / \partial \mathbf{v}$. Writing out carefully the Lagrangian corresponding to the expression for the action S gives:

$$L = -\frac{1}{\gamma(v)} mc^2 - e(\phi - \mathbf{v} \cdot \mathbf{A}), \tag{2.71}$$

from which

$$\mathbf{p}^{\text{canonical}} = \gamma m \mathbf{v} + e\mathbf{A}. \tag{2.72}$$

This gives an elegant form for the action of a particle interacting with an electromagnetic field,

$$S = -\int p_\mu^{\text{canonical}} \, \mathrm{d}x^\mu \,, \tag{2.73}$$

exactly as in the free particle case, except that the canonical momentum has to be written in terms of the velocity and potential using

$$p_\mu^{\text{canonical}} = \gamma(v) m \frac{\mathrm{d}x_\mu}{\mathrm{d}t} + eA_\mu. \tag{2.74}$$

2.4.3 Lagrangian vs. Hamiltonian Methods

Something you might like to check is how the Hamiltonian comes out from the relativistic Lagrangian above; it is of course a time-like quantity and not in any sense frame invariant. Hamilton's equations, because they are equations of *motion*, involve time and hence the particular frame of reference quite explicitly.

Although the Lagrangian is not itself frame independent either, the Lagrangian formulation is frame-invariant. The quantity

$$S[x^\mu(t)] = \int L \, \mathrm{d}t = -\int p_\mu \, \mathrm{d}x^\mu \,, \tag{2.75}$$

is a functional of the path $x^\mu(t)$ which is frame-invariant, as is the variational condition $\delta S = 0$.

Chapter 3

Classical Fields

Much of modern theoretical physics is, one way or another, field theory, the first example of which is the Maxwell approach to electromagnetism. Our next step is into Lagrangians depending on 'fields' rather than 'particle coordinates'. For simplicity we will start with a non-relativistic case, picking up electromagnetism as a relativistic example towards the end.

3.1 Waves in One Dimension

The basic idea is a very simple adaptation of the standard Lagrangian problem. Consider for example the longitudinal modes of an elastic rod (i.e. sound waves in one dimension). Each material point x has a displacement $\varphi(x,t)$; the *dynamical variables* are the φ, one for each value of x, the coordinate values x playing the role of labels on these (infinite number of) physical degrees of freedom.

We can write the kinetic energy as

$$T = \int \frac{1}{2}\rho\left(\frac{\partial\varphi}{\partial t}\right)^2 \mathrm{d}x\,, \tag{3.1}$$

where ρ is the mass per unit length, and the (elastic) potential energy as

$$V = \int \kappa\left(\frac{\partial\varphi}{\partial x}\right)^2 \mathrm{d}x\,, \tag{3.2}$$

where κ is (Young's Modulus)$\times$(cross-sectional area). Indeed, if we modelled this rod as a set of point masses connected by springs, each of potential energy $\frac{1}{2}K(\Delta x)^2$, we would express the total potential energy as a sum of Hookean contributions for each spring, stretched by the relative amount measured by the local displacements $\varphi(x)$:

$$V = \sum_{\{x\}} \frac{1}{2}K[\varphi(x+\delta x)-\varphi(x)]^2 \quad \Longrightarrow \quad \int \frac{1}{2}\kappa\left(\frac{\partial\varphi}{\partial x}\right)^2 \mathrm{d}x\,, \tag{3.3}$$

after transforming the discrete sum into a continuum integral and setting $\kappa = \lim_{\delta x\to 0} K\cdot\delta x$. We can now write down the Lagrangian and action, both as functionals of the **field** $\varphi(x,t)$, respectively

$$L = T - V = \int \left[\frac{1}{2}\rho\left(\frac{\partial\varphi}{\partial t}\right)^2 - \frac{1}{2}\kappa\left(\frac{\partial\varphi}{\partial x}\right)^2\right]\mathrm{d}x \equiv \int \mathcal{L}\,\mathrm{d}x\,, \tag{3.4}$$

$$\text{and,}\quad S = \int L\,\mathrm{d}t = \int \mathcal{L}\,\mathrm{d}x\,\mathrm{d}t\,, \tag{3.5}$$

where $\mathcal{L}$ is the **Lagrangian density**. We use the term 'field' here in the general sense of a function of space and time. The Lagrangian density is a function of the field φ and its derivatives:

$$\mathcal{L}\left(\varphi, \frac{\partial\varphi}{\partial t}, \frac{\partial\varphi}{\partial x}\right) = \frac{1}{2}\rho\left(\frac{\partial\varphi}{\partial t}\right)^2 - \frac{1}{2}\kappa\left(\frac{\partial\varphi}{\partial x}\right)^2. \tag{3.6}$$

The Euler-Lagrange equations from the condition of minimal action $\delta S = 0$ for this type of problem are a straightforward generalisation of the case where we had variables depending on t only. For brevity, write

$$\frac{\partial\varphi}{\partial t} = \dot{\varphi}, \quad \frac{\partial\varphi}{\partial x} = \varphi'. \tag{3.7}$$

For a small variation of the field, $\delta\varphi$, we have

$$\delta S = \int \left(\frac{\partial\mathcal{L}}{\partial\varphi}\delta\varphi + \frac{\partial\mathcal{L}}{\partial\varphi'}\delta\varphi' + \frac{\partial\mathcal{L}}{\partial\dot{\varphi}}\delta\dot{\varphi} \right) \mathrm{d}x\,\mathrm{d}t\,. \tag{3.8}$$

But

$$\int \frac{\partial\mathcal{L}}{\partial\varphi'}\delta\varphi'\,\mathrm{d}x = \int \frac{\partial\mathcal{L}}{\partial\varphi'}\frac{\partial}{\partial x}\delta\varphi\,\mathrm{d}x = \left[\frac{\partial\mathcal{L}}{\partial\varphi'}\delta\varphi\right]_{-\infty}^{+\infty} - \int \frac{\partial}{\partial x}\left(\frac{\partial\mathcal{L}}{\partial\varphi'}\right)\delta\varphi\,\mathrm{d}x\,. \tag{3.9}$$

Just as in the ordinary Lagrangian problem, there are conditions which require the integrated term to vanish. In this case, for the action integral to exist we require the displacement φ, and hence also $\delta\varphi$, to vanish at $x = \pm\infty$. Similarly, for the motion in the time interval $[t_1, t_2]$,

$$\int \frac{\partial\mathcal{L}}{\partial\dot{\varphi}}\delta\dot{\varphi})\,\mathrm{d}t = \left[\frac{\partial\mathcal{L}}{\partial\dot{\varphi}}\delta\varphi\right]_{t_1}^{t_2} - \int \frac{\partial}{\partial t}\left(\frac{\partial\mathcal{L}}{\partial\dot{\varphi}}\right)\delta\varphi\,\mathrm{d}t\,. \tag{3.10}$$

We are interested in minimising the action for given initial and final configurations $\varphi(x, t_1)$ and $\varphi(x, t_2)$, so $\delta\varphi(x, t_{1,2}) = 0$ and again the integrated term vanishes, giving

$$\delta S = \int \left[\frac{\partial\mathcal{L}}{\partial\varphi} - \frac{\partial}{\partial x}\left(\frac{\partial\mathcal{L}}{\partial\varphi'}\right) - \frac{\partial}{\partial x}\left(\frac{\partial\mathcal{L}}{\partial\dot{\varphi}}\right)\right]\delta\varphi\,\mathrm{d}x\,\mathrm{d}t\,. \tag{3.11}$$

This has to vanish for any $\delta\varphi(x, t) = 0$ satisfying the boundary conditions, so we obtain the Euler-Lagrange equation of motion for the field $\varphi(x, t)$:

$$\frac{\partial\mathcal{L}}{\partial\varphi} - \frac{\partial}{\partial x}\left(\frac{\partial\mathcal{L}}{\partial\varphi'}\right) - \frac{\partial}{\partial x}\left(\frac{\partial\mathcal{L}}{\partial\dot{\varphi}}\right) = 0. \tag{3.12}$$

Applying this to our example, we have

$$\mathcal{L} = \frac{1}{2}\rho\dot{\varphi}^2 - \frac{1}{2}\kappa\varphi'^2, \tag{3.13}$$

and so we obtain

$$0 + \frac{\partial}{\partial x}\kappa\varphi' - \frac{\partial}{\partial t}\rho\dot{\varphi} = 0, \tag{3.14}$$

which is just the one dimensional wave equation, as we should have expected. Indeed, writing it in a more familiar format, we recognise both the equation and its solution:

$$\frac{\partial^2\varphi}{\partial t^2} = \frac{\kappa}{\rho}\frac{\partial^2\varphi}{\partial x^2}, \quad \varphi \propto e^{i(\omega t - kx)}, \tag{3.15}$$

with dispersion relation

$$\omega = \sqrt{\frac{\kappa}{\rho}}k. \tag{3.16}$$

We can define a **canonical momentum density**, by analogy with $p = \partial L/\partial v$, as

$$\pi(x, t) = \frac{\partial\mathcal{L}}{\partial\dot{\varphi}} = \rho\dot{\varphi}, \tag{3.17}$$

in our example. This is sensibly analogous to our previous ideas about momentum, in particular, $p = \int \pi \, \mathrm{d}x$. In a system obeying translational invariance, when L does not explicitly depend on q_i (that is, on φ in our example), we would by analogy expect to find the momentum conservation law, although it now involves a more complicated quantity. For $\partial\mathcal{L}/\partial\varphi = 0$, our generalised Euler-Lagrange equation reads

$$\frac{\partial}{\partial t}\pi(x,t) + \frac{\partial}{\partial x}J(x,t) = 0, \tag{3.18}$$

where $J(x,t) = \partial\mathcal{L}/\partial\varphi'$ can be interpreted as the current of canonical momentum. Since $\pi(x,t)$ was the density of canonical momentum, this is just the statement that canonical momentum overall is conserved. In fact, we see that the Euler-Lagrange equation (3.12) or (3.18) for the equilibrium trajectory $\varphi(x,t)$ is the equation for momentum conservation, or the balance of local forces. If you think about balls and springs, we have arrived at the obvious result that the springs cause exchange of momentum between particles (i.e. current of momentum) but conserve momentum overall.

Again in close analogy with particle mechanics, we can define the **Hamiltonian density** $\mathcal{H}$,

$$\mathcal{H}(\varphi, \varphi', \pi) = \pi\dot{\varphi} - \mathcal{L}, \tag{3.19}$$

where $\dot{\varphi}$ is replaced by π as an independent variable. In the case of the elastic rod, this gives

$$\mathcal{H} = \frac{\pi^2}{2\rho} + \frac{1}{2}\kappa\varphi'^2, \tag{3.20}$$

which (since the kinetic energy is a homogeneous quadratic function of $\dot{\varphi}$) is just the total energy density.

3.2 Multidimensional Space

Consider now the extension of this to several dimensions of space, but keeping the physical field $\varphi(\mathbf{x},t)$ as a scalar for the present. We have

$$S = \iint \cdots \int \mathcal{L}\left(\varphi, \frac{\partial\varphi}{\partial t}, \boldsymbol{\nabla}\varphi\right) \mathrm{d}t \, \mathrm{d}x_1 \cdots \mathrm{d}x_d \,, \tag{3.21}$$

and the Euler-Lagrange equation for $\delta S = 0$ gives us

$$\frac{\partial\mathcal{L}}{\partial\varphi} = \frac{\partial}{\partial t}\frac{\partial\mathcal{L}}{\partial(\partial\varphi/\partial t)} + \frac{\partial}{\partial x_1}\frac{\partial\mathcal{L}}{\partial(\partial\varphi/\partial x_1)} + \cdots + \frac{\partial}{\partial x_d}\frac{\partial\mathcal{L}}{\partial(\partial\varphi/\partial x_d)}, \tag{3.22}$$

or if one wants to be more succinct about the spatial derivatives,

$$\frac{\partial\mathcal{L}}{\partial\varphi} = \frac{\partial}{\partial t}\left(\frac{\partial\mathcal{L}}{\partial(\partial\varphi/\partial t)}\right) + \boldsymbol{\nabla}\cdot\left(\frac{\partial\mathcal{L}}{\partial(\boldsymbol{\nabla}\varphi)}\right). \tag{3.23}$$

Note that we still have just one such equation, for the single physical field $\varphi(\mathbf{x},t)$ – the result of having several spatial coordinates is the multicomponent gradient on the r.h.s. The momentum density is also a scalar function, the definition (3.17) remains valid.

The condition of momentum conservation in the case when no external forces are applied, $\partial\mathcal{L}/\partial\varphi = 0$, now resembles the so-called continuity equation:

$$\dot{\pi}(\mathbf{x},t) + \boldsymbol{\nabla}\cdot\mathbf{J}(\mathbf{x},t) = 0, \quad \text{with the vector} \quad \mathbf{J} = \frac{\partial\mathcal{L}}{\partial(\boldsymbol{\nabla}\varphi)}. \tag{3.24}$$

Now it should be fairly obvious that we have in fact put time t and space $\mathbf{x}$ on the same footing, and we can simply regard time (strictly speaking, ct) as one of the coordinate variables x^μ to give

$$\frac{\partial\mathcal{L}}{\partial\varphi} = \frac{\partial}{\partial x^\mu}\left(\frac{\partial\mathcal{L}}{\partial(\,\partial\varphi/\partial x^\mu\,)}\right) \equiv \partial_\mu \frac{\partial\mathcal{L}}{\partial[\partial_\mu\varphi]}, \tag{3.25}$$

(recall that ∂_μ is shorthand for $\partial/\partial x^\mu$) as the Euler-Lagrange equation for the minimal-action condition. Here we are assuming Greek indices to run over time and space and repeated indices in the same expression are summed, just as in relativity. However it should be stressed that our equations are in no way particular to Special Relativity - though of course they very naturally encompass it, as we now explore in more detail.

3.3 Relativistic Scalar Field

In Special Relativity the action S is a Lorentz invariant quantity and Eq. (3.21) involves an integration with respect to the invariant space-time volume element $\mathrm{d}^4x = c\,\mathrm{d}t\,\mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z$. It follows that the Lagrangian density $\mathcal{L}$ is also a Lorentz invariant (scalar) function. If we require that the Euler-Lagrange equation of motion for the field be linear and at most a second-order differential equation, this limits $\mathcal{L}$ to the general form

$$\mathcal{L} = \alpha(\partial^\mu\varphi)(\partial_\mu\varphi) + \beta\partial^\mu\partial_\mu\varphi + \gamma\varphi\partial^\mu\partial_\mu\varphi + \delta\varphi + \epsilon\varphi^2, \tag{3.26}$$

where α, β, γ, δ and ϵ are *constants*. Writing this as

$$\mathcal{L} = (\alpha-\gamma)(\partial^\mu\varphi)(\partial_\mu\varphi) + \partial^\mu(\beta\partial_\mu\varphi + \gamma\varphi\partial_\mu\varphi) + \delta\varphi + \epsilon\varphi^2, \tag{3.27}$$

we note that the total derivative term $\partial^\mu(\cdots)$ can be integrated to give a (4D) surface contribution to the action, which does not affect the equation of motion since the field vanishes at infinite distance and is fixed in the distant past and future. Furthermore the equation of motion is unaffected by an overall rescaling of the action, so we may as well choose $\alpha - \gamma = \frac{1}{2}$. Thus the most general physically significant form is

$$\mathcal{L} = \frac{1}{2}(\partial^\mu\varphi)(\partial_\mu\varphi) + \delta\gamma + \epsilon\gamma^2. \tag{3.28}$$

which leads to the equation of motion

$$\partial^\mu\partial_\mu\varphi - \delta - 2\epsilon\varphi = 0. \tag{3.29}$$

(To get the first term, write $(\partial^\mu\varphi)(\partial_\mu\varphi) = g^{\mu\nu}(\partial_\nu\varphi)(\partial_\mu\varphi)$ and note that both derivatives contribute to the r.h.s. of Eq. (3.25) because of the summation convention.)

According to the boundary conditions, $\varphi = 0$ at infinity and therefore we must have $\delta = 0$. Finally, we shall see shortly that ϵ must be negative, so it is convenient to redefine

$\epsilon = -m^2/2$. In summary, the most general acceptable Lagrangian density for a real scalar field with linear dynamics is

$$\mathcal{L} = \frac{1}{2}(\partial^\mu\varphi)(\partial_\mu\varphi) - \frac{1}{2}m^2\varphi^2, \tag{3.30}$$

with the **Klein-Gordon** equation of motion,

$$\partial^\mu\partial_\mu\varphi + m^2\varphi = 0. \tag{3.31}$$

Writing out the Lagrangian density (3.30) in more detail,

$$\mathcal{L} = \frac{1}{2c^2}\left(\frac{\partial\varphi}{\partial t}\right)^2 - \frac{1}{2}(\boldsymbol{\nabla}\varphi)^2 - \frac{1}{2}m^2\varphi^2, \tag{3.32}$$

we see that the momentum density is

$$\pi = \frac{\partial\mathcal{L}}{\partial\dot{\varphi}} = \frac{1}{c^2}\frac{\partial\varphi}{\partial t}, \tag{3.33}$$

and so the Klein-Gordon Hamiltonian density is

$$\mathcal{H} = \frac{1}{2}c^2\pi^2 + \frac{1}{2}(\boldsymbol{\nabla}\varphi)^2 + \frac{1}{2}m^2\varphi^2. \tag{3.34}$$

This quantity is positive-definite if and only if the coefficient of φ^2 is positive. If the coefficient were negative, there would be field configurations with arbitrarily large negative energy, and the system would have no stable ground state. This justifies our decision to write the coefficient $(-\epsilon)$ as $m^2/2$.

3.4 Natural units

In dealing with relativistic systems it is convenient to use units such that $c = 1$. Then lengths are measured in the same units as times (the time it takes light to travel that distance), and mass in the same units as energy (the energy released by annihilating that mass). In these units Eqs. (3.32) and (3.34) become

$$\mathcal{L} = \frac{1}{2}\left(\frac{\partial\varphi}{\partial t}\right)^2 - \frac{1}{2}(\boldsymbol{\nabla}\varphi)^2 - \frac{1}{2}m^2\varphi^2, \tag{3.35}$$

$$\mathcal{H} = \frac{1}{2}\pi^2 + \frac{1}{2}(\boldsymbol{\nabla}\varphi)^2 + \frac{1}{2}m^2\varphi^2, \tag{3.36}$$

since now $\pi = \partial\varphi/\partial t$.

However, these units are still not optimal since $\mathcal{L}$ and $\mathcal{H}$ are supposed to have the dimensions of energy density, which in $c = 1$ units ($[L] = [T]$) are $[M][T]^{-3}$. That would mean that φ has to have dimensions $[M]^{1/2}[T]^{-1/2}$. Since in practice we are dealing with fields that represent phenomena on the subatomic scale, it is simplest to couple the dimensions of energy/mass and time as well, by using units in which $\hbar = c = 1$. Since $[\hbar] = [E][T]$ this means that time is measured in units of inverse energy or mass (the energy of a quantum whose angular frequency is the inverse of that time). These are called *natural units*, at least by particle physicists. For them the natural scale of energy is

measured in giga-electron-volts, GeV. Then the magic formula for converting to everyday units is

$$\hbar c = 0.2 \text{ GeV fm}, \tag{3.37}$$

where 1 fm (femtometre) is 10^{-15} m.

In natural units, $[T] = [E]^{-1} = [M]^{-1}$ and the dimensions of $\mathcal{L}$ and $\mathcal{H}$ are $[M]^4$, so φ has simply dimensions of mass. You can check that every term in Eq. (3.36) has dimension $[M]^4$, provided the constant m is itself interpreted as a mass.

We shall usually employ natural units in this section from now on. With a little practice, it is straightforward to reinsert the correct number of factors of $\hbar$ and c to convert any given expression into SI units.

3.5 Fourier Analysis

Consider first, for simplicity, solutions of the Klein-Gordon equation that depend only on x and t. They satisfy the 1-dimensional version of Eq. (3.31), i.e. (in natural units)

$$\frac{\partial^2\varphi}{\partial t^2} - \frac{\partial^2\varphi}{\partial x^2} + m^2\varphi = 0. \tag{3.38}$$

We can express any real field $\varphi(x,t)$ as a Fourier integral:

$$\varphi(x,t) = \int \mathrm{d}k\, N(k)\Big[a(k)e^{i(kx-\omega t)} + a^*(k)e^{-i(kx-\omega t)}\Big], \tag{3.39}$$

where $N(k)$ is a convenient normalizing factor for the Fourier transform $a(k)$, which we choose to satisfy $N(-k) = N(k)$ for later convenience. The frequency $\omega(k)$ is obtained by solving the equation of motion: the Klein-Gordon equation gives $\omega^2 = k^2 + m^2$ and therefore

$$\omega = +\sqrt{k^2+m^2}, \tag{3.40}$$

where we choose the positive root because Eq. (3.39) includes $+\omega$ and $-\omega$ explicitly. The Hamiltonian

$$H = \int \left(\frac{1}{2}\pi^2 + \frac{1}{2}\varphi'^2 + \frac{1}{2}m^2\varphi^2\right)\mathrm{d}x \tag{3.41}$$

takes a simpler form in terms of the Fourier amplitudes $a(k)$. We can write e.g.

$$\varphi^2 = \int \mathrm{d}k\, N(k)[\cdots] \int \mathrm{d}k'\, N(k')[\cdots], \tag{3.42}$$

and use

$$\int \mathrm{d}x\, e^{i(k\pm k')x} = 2\pi\delta(k \pm k') \tag{3.43}$$

to show that

$$\int \varphi^2\,\mathrm{d}x = 2\pi \int \mathrm{d}k\,\mathrm{d}k'\, N(k)N(k')\Big[a(k)a(k')\delta(k+k')e^{-i(\omega+\omega')t} + a^*(k)a^*(k')\delta(k+k')e^{i(\omega+\omega')t} + a(k)a^*(k')\delta(k-k')e^{-i(\omega-\omega')t} + a^*(k)a(k')\delta(k-k')e^{i(\omega-\omega')t}\Big] \tag{3.44}$$

Noting that $\omega(-k) = \omega(k)$ and with the choice $N(-k) = N(k)$, this gives

$$\int \varphi^2 \, \mathrm{d}x = 2\pi \int \mathrm{d}k \, [N(k)]^2 \Big[a(k)a(-k)e^{-2i\omega t} + a^*(k)a^*(-k)e^{2i\omega t} + a(k)a^*(k) + a^*(k)a(k) \Big]. \tag{3.45}$$

Similarly,

$$\int \varphi'^2 \, \mathrm{d}x = 2\pi \int \mathrm{d}k \, [kN(k)]^2 \Big[a(k)a(-k)e^{-2i\omega t} + a^*(k)a^*(-k)e^{2i\omega t} + a(k)a^*(k) + a^*(k)a(k) \Big], \tag{3.46}$$

while,

$$\int \dot{\varphi}^2 \, \mathrm{d}x = 2\pi \int \mathrm{d}k \, [\omega(k)N(k)]^2 \Big[-a(k)a(-k)e^{-2i\omega t} - a^*(k)a^*(-k)e^{2i\omega t} + a(k)a^*(k) + a^*(k)a(k) \Big]. \tag{3.47}$$

and hence, using $k^2 = \omega^2 - m^2$,

$$H = 2\pi \int \mathrm{d}k \, [N(k)\omega(k)]^2 \Big[a(k)a^*(k) + a^*(k)a(k) \Big], \tag{3.48}$$

or, choosing

$$N(k) = \frac{1}{2\pi \cdot 2\omega(k)}, \tag{3.49}$$

$$H = \int \mathrm{d}k \, N(k) \frac{1}{2} \omega(k) \Big[a(k)a^*(k) + a^*(k)a(k) \Big], \tag{3.50}$$

i.e. the integrated *density of modes* $N(k)$ times the *energy per mode* $\omega(k)|a(k)|^2$.

Hence each normal mode of the system behaves like an independent harmonic oscillator with amplitude $a(k)$.

In 3 spatial dimensions we write

$$\varphi(\mathbf{r}, t) = \int \mathrm{d}^3\mathbf{k} \, N(\mathbf{k}) \Big[a(\mathbf{k}) e^{i(\mathbf{k}\cdot\mathbf{r} - \omega t)} + a^*(\mathbf{k}) e^{-i(\mathbf{k}\cdot\mathbf{r} - \omega t)} \Big], \tag{3.51}$$

and use

$$\int \mathrm{d}^3\mathbf{r} \, e^{i(\mathbf{k} \pm \mathbf{k}')\cdot\mathbf{r}} = (2\pi)^3 \delta^3(\mathbf{k} \pm \mathbf{k}'). \tag{3.52}$$

Therefore we should choose

$$N(\mathbf{k}) = \frac{1}{(2\pi)^3 2\omega(\mathbf{k})} \tag{3.53}$$

to obtain an integral with the usual relativistic phase space (density of states) factor:

$$H = \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3 2\omega(\mathbf{k})} \omega(\mathbf{k}) |a(\mathbf{k})|^2. \tag{3.54}$$

3.6 Multi-Component Fields

We now look at examples where the field itself has a more complicated structure. In principle, there is no significant difference and the analogies we have been observing will continue to hold, if each component of the physical field is regarded as an independent scalar variable as was studied above. Let us consider first an example with an intuitively clear 2-dimensional vector field.

3.6.1 Transverse Waves on a String

Instead of longitudinal modes of a rod, consider small transverse displacements $\boldsymbol{\varphi} = (\varphi_y, \varphi_z)$ of a flexible elastic string stretched along the x-axis at constant tension F. Then the kinetic energy is

$$T = \frac{1}{2}\rho \int \left[\left(\frac{\partial \varphi_y}{\partial t} \right)^2 + \left(\frac{\partial \varphi_z}{\partial t} \right)^2 \right] \mathrm{d}x \,, \tag{3.55}$$

and the elastic potential energy is

$$\begin{aligned} V = F\left[\int \mathrm{d}s - \int \mathrm{d}x \right] &= F \int \left[\sqrt{1 + \left(\frac{\partial \varphi_y}{\partial x} \right)^2 + \left(\frac{\partial \varphi_z}{\partial x} \right)^2} - 1 \right] \mathrm{d}x \\ &= \frac{1}{2} F \int \left[\left(\frac{\partial \varphi_y}{\partial x} \right)^2 + \left(\frac{\partial \varphi_z}{\partial x} \right)^2 \right] \mathrm{d}x \,, \end{aligned} \tag{3.56}$$

for small displacements (and small displacement gradients). Therefore the Lagrangian density just becomes

$$\mathcal{L} = \frac{1}{2} \sum_{j-y,z} \left[\rho \left(\frac{\partial \varphi_j}{\partial t} \right)^2 - F \left(\frac{\partial \varphi_j}{\partial x} \right)^2 \right]. \tag{3.57}$$

The action is to be mimimised with respect to variations in both φ_y and φ_z, so we now get Euler-Lagrange conditions for each component:

$$\frac{\partial \mathcal{L}}{\partial \varphi_j} = \frac{\partial}{\partial t} \left(\frac{\partial \mathcal{L}}{\partial (\partial \varphi_j / \partial t)} \right) + \frac{\partial}{\partial x} \left(\frac{\partial \mathcal{L}}{\partial (\partial \varphi_j / \partial x)} \right), \tag{3.58}$$

which in this case give identical wave equations for $j = y$ and z:

$$0 = \frac{\partial}{\partial t} \rho \left(\frac{\partial \varphi_j}{\partial t} \right) - \frac{\partial}{\partial x} F \left(\frac{\partial \varphi_j}{\partial x} \right). \tag{3.59}$$

Thus transverse waves propagate with velocity $\sqrt{F/p}$, independent of the direction of the displacement vector φ, i.e. independent of their *polarisation*.

For a multi-component field in multidimensional space we again have to regard each component of the vector field φ as a separate field giving us an Euler-Lagrange condition for each of these components:

$$\frac{\partial \mathcal{L}}{\partial \varphi_j} = \frac{\partial}{\partial t} \left(\frac{\partial \mathcal{L}}{\partial (\partial \varphi_j / \partial t)} \right) + \boldsymbol{\nabla} \cdot \left(\frac{\partial \mathcal{L}}{\partial (\boldsymbol{\nabla} \varphi_j)} \right). \tag{3.60}$$

For example, in the case of elastic waves in a three-dimensional medium, $\boldsymbol{\varphi}$ represents the displacement of a material point in the medium and Eq. (3.60) leads to the **acoustic wave equation**. For a general medium, the wave velocity now depends on the polarization, but the details of this would take us too far into the theory of elasticity.

3.7 Complex Scalar Field

Suppose φ is a complex scalar field, i.e. $\varphi^* \neq \varphi$. We can always decompose it into

$$\varphi = \frac{1}{\sqrt{2}} (\varphi_1 + i\varphi_2), \tag{3.61}$$

where φ_1 and φ_2 are real. Then, writing φ_1 and φ_2 as Fourier integrals as in Eq. (3.39),

$$\varphi(x,t) = \int \mathrm{d}k\, N(k)\Big[a(k)e^{i(kx-\omega t)} + b^*(k)e^{-i(kx-\omega t)}\Big], \tag{3.62}$$

where

$$a = \frac{1}{\sqrt{2}}(a_1 + ia_2), \quad b^* = \frac{1}{\sqrt{2}}(a_1^* + ia_2^*) \neq a^*. \tag{3.63}$$

The Lagrangian density

$$\mathcal{L} = \mathcal{L}[\varphi_1] + \mathcal{L}[\varphi], \tag{3.64}$$

can be written as

$$\mathcal{L} = \frac{\partial\varphi^*}{\partial t}\frac{\partial\varphi}{\partial t} - \frac{\partial\varphi^*}{\partial x}\frac{\partial\varphi}{\partial x} - m^2\varphi^*\varphi. \tag{3.65}$$

The canonical momentum densities conjugate to φ and φ^* are thus

$$\pi = \frac{\partial\mathcal{L}}{\partial\dot{\varphi}} = \frac{\partial\varphi^*}{\partial t}, \quad \pi^* = \frac{\partial\mathcal{L}}{\partial\dot{\varphi}^*} = \frac{\partial\varphi}{\partial t}, \tag{3.66}$$

and the Hamiltonian density is

$$\mathcal{H} = \pi\dot{\varphi} + \pi^*\dot{\varphi}^* - \mathcal{L} = \pi^*\pi + \frac{\partial\varphi^*}{\partial x}\frac{\partial\varphi}{\partial x} + m^2\varphi^*\varphi. \tag{3.67}$$

Using the Fourier expansion of φ and integrating over all space (left as an exercise!), we find

$$\begin{aligned} H = \int \mathrm{d}x\,\mathcal{H} &= \frac{1}{2}\int \mathrm{d}k\, N(k)\omega(k)\Big[a(k)a^*(k) + a^*(k)a(k) + b(k)b^*(k) + b^*(k)b(k)\Big] \\ &= \int \mathrm{d}k\, N(k)\omega(k)\Big[|a(k)|^2 + |b(k)|^2\Big]. \end{aligned} \tag{3.68}$$

Therefore the positive and negative frequency Fourier components of the field contribute to the energy with the same (positive) sign.

In 3 spatial dimensions Eq. (3.65) becomes

$$\begin{aligned} \mathcal{L} &= \frac{\partial\varphi^*}{\partial t}\frac{\partial\varphi}{\partial t} - \boldsymbol{\nabla}\varphi^*\cdot\boldsymbol{\nabla}\varphi - m^2\varphi^*\varphi \\ &= \partial_\mu\varphi^*\partial^\mu\varphi - m^2\varphi^*\varphi, \end{aligned} \tag{3.69}$$

and the Fourier decomposition of the field is

$$\varphi = \int \mathrm{d}^3\mathbf{k}\, N(\mathbf{k})\Big[a(\mathbf{k})e^{-ik\cdot x} + b^*(\mathbf{k})e^{ik\cdot x}\Big] \tag{3.70}$$

where $N(\mathbf{k})$ is given by Eq. (3.53) and for brevity we have introduced the wave 4-vector $k^\mu = (\omega/c, \mathbf{k})$ in the exponents, so that

$$k\cdot x = k^\mu x_\mu = \omega t - \mathbf{k}\cdot\mathbf{r}. \tag{3.71}$$

Then in place of (3.68) we have

$$H = \int \mathrm{d}^3\mathbf{k}\, N(\mathbf{k})\omega(\mathbf{k})\Big[|a(\mathbf{k})|^2 + |b(\mathbf{k})|^2\Big]. \tag{3.72}$$

3.8 Electromagnetic Field

Finally, let us have a look at the electromagnetic field, although this is a much more difficult and involved subject! The starting point has to be the four-potential A_μ in terms of which the physical fields $\mathbf{E}$ and $\mathbf{B}$ can be found (with a bit of effort) amongst the components of the electromagnetic field strength tensor

$$F_{\alpha\beta} = \partial_\alpha A_\beta - \partial_\beta A_\alpha \quad \text{or} \quad F_{\alpha\beta} = \begin{pmatrix} 0 & E_x/c & E_y/c & E_z/c \\ -E_x/c & 0 & -B_z & B_y \\ -E_y/c & B_z & 0 & -B_x \\ -E_z/c & -B_y & B_x & 0 \end{pmatrix}. \tag{3.73}$$

Note that $F_{\alpha\beta}$ is antisymmetric (and therefore has zero diagonal elements). This is an example of a physical variable expressed by a second-rank tensor field. Now one needs to construct the appropriate Lagrangian density from it.

As we already discussed for the relativistic scalar field, given that the Lagrangian action S is a frame invariant scalar, it follows we should expect the Lagrangian density $\mathcal{L}$ to be a scalar also. This rather limits the possibilities of how we could construct $\mathcal{L}$ from the traceless second-rank tensor $F_{\alpha\beta}$.

We want $\mathcal{L}$ to be a scalar, and to give us Euler-Lagrange equations which are linear in the physical fields $\mathbf{E}$ and $\mathbf{B}$ (the components of $F_{\alpha\beta}$). Therefore, we need $\mathcal{L}$ to be at most quadratic in these components and the only possible form is $\mathcal{L}_0 = aF_{\alpha\beta}F^{\alpha\beta}$ (a linear term, if it existed, would have to be the trace of $F^{\alpha\beta}$, which is zero by construction). This is the first level of approximation, corresponding to Maxwell electromagnetism. Extensions could arise, for instance, by bringing in spatial gradients: squared powers of $\partial_\mu F^{\alpha\beta}$ would lead to a variety of effects such as spatial dispersion, optical rotation, etc. Let us stay on the most basic level here.

In view of what we found for the single relativistic particle, it is evidently prudent to anticipate the coupling of the free field $F^{\alpha\beta}$ to the electric current distribution, characterised by the four-current J^μ, defined as $\rho(\mathrm{d}x^\mu/\mathrm{d}t)$ with ρ the charge density. The timelike component of J^μ is just the charge density (with a factor c), while the spacelike components are $\rho\mathbf{v} \equiv \mathbf{J}$, the density of electric current. This corresponds to the external force term in the potential energy of the elastic Lagrangians in the preceding examples and, in general, leads to a non-zero l.h.s. in the corresponding Euler-Lagrange equations, such as (3.12) and (3.60). In the electromagnetic field case this then leads us to consider the Lagrangian density

$$\mathcal{L} = aF_{\alpha\beta}F^{\alpha\beta} - J^\mu A_\mu. \tag{3.74}$$

Another important constraint in electromagnetism, which we have already discussed in Section 2.3, is gauge invariance: we can let $a_\mu \to A_\mu + \partial_\mu f$ (in 4-vector notation), where f is any scalar function, without altering the physical fields $F_{\alpha\beta}$. Evidently our Lagrangian density with the coupling to an external current is not gauge invariant, but if you compute the corresponding change in the action S you find

$$\Delta S = -\int J^\mu(\partial_\mu f)\,\mathrm{d}^4x = +\int f(\partial_\mu J^\mu)\,\mathrm{d}^4x + (\text{boundary current terms}), \tag{3.75}$$

and the r.h.s. vanishes if the current J^μ is conserved, that is if the 4-gradient $\partial_\mu J^\mu = 0$ (and if the current does not flow out through the boundaries). Therefore coupling the

vector potential to conserved currents leaves the Lagrangian Action (but not $\mathcal{L}$) gauge invariant.

Now we have to check that all this really works, that is, it leads to real electromagnetism. For instance, let us check that we do get Maxwell's equations for the field components! Clearly, they have to satisfy the minimal-action condition, i.e. to be the relevant Euler-Lagrange equations. All we need to do is to rewrite the canonical form in an appropriate way.

Let us take the four-potential A_μ as the basic field variable of the Euler-Lagrange equations for $\delta S = 0$. We have then

$$\frac{\partial \mathcal{L}}{\partial A_\alpha} = \frac{\partial}{\partial x^\mu}\left(\frac{\partial \mathcal{L}}{\partial(\partial_\mu A_\alpha)}\right), \tag{3.76}$$

and the l.h.s. immediately gives $-J^\alpha$, the external "force". For the r.h.s. we need to calculate the derivative

$$\frac{\partial}{\partial(\partial_\mu A_\alpha)} a F_{\delta\gamma} F^{\delta\gamma} = a F^{\delta\gamma} \frac{\partial}{\partial(\partial_\mu A_\alpha)} F_{\delta\gamma} + a F_{\delta\gamma} \frac{\partial}{\partial(\partial_\mu A_\alpha)} F^{\delta\gamma}. \tag{3.77}$$

It is not too hard to convince yourself that the two terms are in fact equal, and that by permuting indices each of these is equal to

$$2a F^{\delta\gamma} \frac{\partial}{\partial(\partial_\mu A_\alpha)} \partial_\delta A_\gamma = 2a F^{\mu\alpha}. \tag{3.78}$$

The Euler-Lagrange equations therefore reduce to the 4-vector relation

$$J^\alpha + 4a \partial_\mu F^{\mu\alpha} = 0, \tag{3.79}$$

or if you prefer

$$J^\alpha + 4a(\partial_\mu \partial^\mu A^\alpha - \partial^\alpha \partial_\mu A^\mu) = 0. \tag{3.80}$$

With a suitable choice of the constant, $a = -1/4\mu_0$, these are just the inhomogeneous pair of Maxwell equations (recall here that $c^2 = 1/\epsilon_0\mu_0$)

$$\boldsymbol{\nabla} \cdot \mathbf{E} = \frac{\rho}{\epsilon_0}, \quad \boldsymbol{\nabla} \times \mathbf{B} = \epsilon_0\mu_0 \frac{\partial \mathbf{E}}{\partial t} + \mu_0 \mathbf{J}. \tag{3.81}$$

The important continuity equation is then obtained by covariant differentiation of (3.79):

$$\partial_\mu \partial_\nu F^{\mu\nu} = 0 = \partial_\nu J^\nu = \mu_0 \left(\frac{\partial \rho}{\partial t} + \boldsymbol{\nabla} \cdot \mathbf{J}\right), \tag{3.82}$$

meaning that the charge is conserved (recall that $F^{\mu\nu}$ is antisymmetric and therefore vanishes whenever both indices are contracted with a symmetric tensor, $\partial_\mu \partial_\nu$ in this case). The other pair of Maxwell equations is actually contained in the definition of the antisymmetric tensor $F^{\mu\nu}$:

$$\partial^\lambda F^{\mu\nu} + \partial^\nu F^{\lambda\mu} + \partial^\mu F^{\nu\lambda} = 0, \tag{3.83}$$

(the so-called *Bianchi identity*). When written out explicitly, this gives $\boldsymbol{\nabla} \cdot \mathbf{B} = \boldsymbol{\nabla} \times \mathbf{E} + \dot{\mathbf{B}} = 0$.

To sum up much of what we have covered regarding the electromagnetic field, the action for the EM field plus charged relativistic particles is given by

$$S = \sum_{\text{particles}} \left[-\int mc^2 \, \mathrm{d}\tau \quad - \int eA_\mu \, \mathrm{d}x^\mu \, (t) \right] - \frac{1}{4\mu_0} \int F_{\alpha\beta} F^{\alpha\beta} \, \mathrm{d}^4 x \, , \tag{3.84}$$

free particles	coupling to EM field	free EM field
Section 2.4	Section 2.3	here

and the condition $\delta S = 0$ gives both the motion of the particles in the field and the dynamics of the field due to the particles. This means that the full relativistic electromagnetic interactions between the particles (retardation, radiation and all) are included, excluding of course quantum mechanical effects.

3.8.1 Gauge Invariance

The gauge transformations (2.53) and (2.54) of the EM potentials are simply expressed in covariant form as

$$A'_\mu = A_\mu + \partial_\mu f. \tag{3.85}$$

The invariance of electromagnetism with respect to this transformation allows us to impose one constraint on A_μ, for example the axial gauge condition $n^\mu A_\mu = 0$, which now includes the choice $\phi = 0$ or $\mathbf{n} \cdot \mathbf{A} = 0$, according to the choice of the arbitrary 4-vector n^μ.

We also already mentioned the Lorenz gauge, where the condition (2.55) in covariant notation becomes $\partial_\mu A^\mu = 0$, which is manifestly Lorentz invariant. Furthermore this choice leaves Eq. (3.80) as simply the wave equation $\partial_\mu \partial^\mu A^\alpha$ in the absence of charges. The residual ambiguity (2.56) in this gauge similarly takes the form $\partial_\mu \partial^\mu f = 0$..

We shall have a good deal more to say about gauge invariance after we have considered in more detail the relationship between symmetries and conservation laws in the next chapter.

Chapter 4

Symmetries and Conservation Laws

The relationship between symmetries and conserved quantities, and the effects of symmetry breaking, are amongst the most important in theoretical physics. We start with the simplest case of the scalar (Klein-Gordon) field, then add electromagnetism. Finally we introduce the transition from classical to quantum fields, which clarifies the interpretation of conserved quantities such as energy and charge.

4.1 Noether's Theorem

Let us try to find a current and a density that satisfy the continuity equation for the complex Klein-Gordon field. We use an important general result called *Noether's theorem* (Emmy Noether, 1918), which tells us that there is a *conserved current* associated with every continuous *symmetry* of the Lagrangian, i.e. with symmetry under a transformation of the form

$$\varphi \to \varphi + \delta\varphi, \tag{4.1}$$

where $\delta\varphi$ is infinitesimal. Symmetry means that $\mathcal{L}$ doesn't change:

$$\delta\mathcal{L} = \frac{\partial\mathcal{L}}{\partial\varphi}\delta\varphi + \frac{\partial\mathcal{L}}{\partial\varphi'}\delta\varphi' + \frac{\partial\mathcal{L}}{\partial\dot{\varphi}}\delta\dot{\varphi} = 0, \tag{4.2}$$

where

$$\delta\varphi' = \delta\left(\frac{\partial\varphi}{\partial x}\right) = \frac{\partial}{\partial x}\delta\varphi \tag{4.3}$$

$$\delta\dot{\varphi} = \delta\left(\frac{\partial\varphi}{\partial t}\right) = \frac{\partial}{\partial t}\delta\varphi \tag{4.4}$$

(easily generalised to 3 spatial dimensions).

The Euler-Lagrange equation of motion

$$\frac{\partial\mathcal{L}}{\partial\varphi} - \frac{\partial}{\partial x}\left(\frac{\partial\mathcal{L}}{\partial\varphi'}\right) - \frac{\partial}{\partial t}\left(\frac{\partial\mathcal{L}}{\partial\dot{\varphi}}\right) = 0, \tag{4.5}$$

then implies that

$$\begin{aligned}\delta\mathcal{L} = \frac{\partial}{\partial x}\left(\frac{\partial\mathcal{L}}{\partial\varphi'}\right)\delta\varphi + \frac{\partial\mathcal{L}}{\partial\varphi'}\frac{\partial}{\partial x}(\delta\varphi) + \frac{\partial}{\partial t}\left(\frac{\partial\mathcal{L}}{\partial\dot{\varphi}}\right)\delta\varphi + \frac{\partial\mathcal{L}}{\partial\dot{\varphi}}\frac{\partial}{\partial t}(\delta\varphi) = 0 \\ \implies \quad \frac{\partial}{\partial x}\left(\frac{\partial\mathcal{L}}{\partial\varphi'}\delta\varphi\right) + \frac{\partial}{\partial t}\left(\frac{\partial\mathcal{L}}{\partial\dot{\varphi}}\delta\varphi\right) = 0.\end{aligned} \tag{4.6}$$

Comparing with the conservation/continuity equation (in 1 dimension)

$$\frac{\partial}{\partial x}(J_x) + \frac{\partial\rho}{\partial t} = 0, \tag{4.7}$$

we see that the conserved density and current are (proportional to)

$$\rho = \frac{\partial \mathcal{L}}{\partial \dot{\varphi}} \delta\varphi, \quad J_x = \frac{\partial \mathcal{L}}{\partial \varphi'} \delta\varphi. \tag{4.8}$$

In 3 spatial dimensions

$$J_x = \frac{\partial \mathcal{L}}{\partial(\,\partial\varphi/\partial x\,)} \delta\varphi, \quad J_y \frac{\partial \mathcal{L}}{\partial(\,\partial\varphi/\partial y\,)} \delta\varphi, \quad \cdots \quad , \tag{4.9}$$

and hence in covariant notation

$$J^\mu = \frac{\partial \mathcal{L}}{\partial(\partial_\mu \varphi)} \delta\varphi. \tag{4.10}$$

If the Lagrangian involves several fields $\varphi_1, \varphi_2, \cdots$, the symmetry may involve changing them all: invariance w.r.t. $\varphi_j \to \varphi_j + \delta\varphi_j$ then implies the existence of a conserved *Noether current*

$$J^\mu = \sum_j \frac{\partial \mathcal{L}}{\partial(\partial_\mu \varphi_j)} \delta\varphi_j. \tag{4.11}$$

In general the transformation may mix the different fields, so that

$$\delta\varphi_j = \varepsilon \sum_k t_{jk} \varphi_k, \tag{4.12}$$

where ε is a small parameter and t_{ik} are constants. Then, dividing out ε, the Noether current is

$$J^\mu = \sum_{j,k} t_{jk} \frac{\partial \mathcal{L}}{\partial(\partial_\mu \varphi_j)} \delta\varphi_k. \tag{4.13}$$

4.2 Global Phase Symmetry

As an important example, consider the Klein-Gordon Lagrangian density for a complex field, Eq. (3.69):

$$\mathcal{L} = \partial_\mu \varphi^* \partial^\mu \varphi - m^2 \varphi^* \varphi. \tag{4.14}$$

This is invariant under a *global phase change* in φ:

$$\varphi \to e^{-i\varepsilon} \varphi \simeq \varphi - i\varepsilon\varphi \tag{4.15}$$

$$\varphi^* \to e^{+i\varepsilon} \varphi^* \simeq \varphi^* + i\varepsilon\varphi^*, \tag{4.16}$$

i.e. $\delta\varphi \propto -i\varphi$, $\delta\varphi^* \propto +i\varphi^*$. By 'global' we mean that the phase change ε is the same at all points in space-time.

The corresponding conserved Noether current is

$$J^\mu = \frac{\partial \mathcal{L}}{\partial(\partial_\mu \varphi)} \delta\varphi + \delta\varphi^* \frac{\partial \mathcal{L}}{\partial(\partial_\mu \varphi^*)} = -i(\partial^\mu \varphi^*)\varphi + i\varphi^*(\partial^\mu \varphi). \tag{4.17}$$

We can define an associated *conserved charge*, which is the integral of ρ over all space:

$$Q = \int \rho \, \mathrm{d}^3\mathbf{r} \,. \tag{4.18}$$

$$\frac{\mathrm{d}Q}{\mathrm{d}t} = \int \frac{\partial \rho}{\partial t} \, \mathrm{d}^3\mathbf{r} = -\int \boldsymbol{\nabla} \cdot \mathbf{J} \, \mathrm{d}^3\mathbf{r} = -\int_{\infty \text{ sphere}} \mathbf{J} \cdot \mathrm{d}\mathbf{S} = 0. \tag{4.19}$$

In this case

$$Q = -i \int \left(\frac{\partial \varphi^*}{\partial t} \varphi - \varphi^* \frac{\partial \varphi}{\partial t} \right) \mathrm{d}^3\mathbf{r} \,. \tag{4.20}$$

Inserting the Fourier decomposition (3.70) for the field,

$$\varphi = \int \mathrm{d}^3\mathbf{r} \, N(\mathbf{k}) \Big[a(\mathbf{k}) e^{-ik\cdot x} + b^*(\mathbf{k}) e^{ik\cdot x} \Big], \tag{4.21}$$

we find (another exercise!)

$$Q = \int \mathrm{d}^3\mathbf{k} \, N(\mathbf{k}) \Big[|a(\mathbf{k})|^2 - |b(\mathbf{k})|^2 \Big]. \tag{4.22}$$

Therefore the positive and negative frequency Fourier components of the field contribute to the charge with *opposite* signs, in contrast to their contributions to the energy. We shall see that, when a complex classical field is quantised, the quanta can be either *particles* (quanta with positive energy and positive charge) or *antiparticles* (quanta with positive energy and negative charge).

4.3 Local Phase (Gauge) Symmetry

Suppose now that we make a *local* phase change in a complex scalar field φ, i.e. we allow the phase ε to be a function of the space-time coordinates x^μ. This is not a symmetry of the free-field Klein-Gordon Lagrangian $\mathcal{L}_{KG}$ because

$$\varphi \to e^{-i\varepsilon(x)} \varphi \implies \partial^\mu \varphi \to e^{-i\varepsilon(x)} [(\partial^\mu \varphi) - i(\partial^\mu \varepsilon)\varphi], \tag{4.23}$$

and therefore

$$\begin{aligned} \mathcal{L}_{KG} &\to [\partial_\mu \varphi^* + i(\partial_\mu \varepsilon)\varphi^*][\partial^\mu \varphi - i(\partial^\mu \varepsilon)\varphi] - m^2 \varphi^* \varphi \\ &= \mathcal{L}_{KG} - i(\partial_\mu \varepsilon)[(\partial^\mu \varphi^*)\varphi - \varphi^*(\partial^\mu \varphi)] + (\partial_\mu \varepsilon)(\partial^\mu \varepsilon)\varphi^* \varphi. \end{aligned} \tag{4.24}$$

Notice that the second term on the r.h.s. is proportional to the current $J^\mu = -i[(\partial^\mu \varphi^*)\varphi - \varphi^*(\partial^\mu \varphi)]$. In the presence of an electromagnetic field this term will cancel with the change in the interaction term $-eJ^\mu A_\mu$ if we make a simultaneous gauge transformation

$$A_\mu \to A_\mu + \partial_\mu \varepsilon / e, \tag{4.25}$$

i.e. we choose the scalar function f in Eq. (3.85) to be ε/e. And in fact the last term will also cancel if we introduce the electromagnetic interaction through the so-called *covariant derivative*

$$\partial_\mu \to D_\mu = \partial_\mu + ieA_\mu, \tag{4.26}$$

for then the combined effect of the phase change in φ and the gauge change in A_μ will be such that

$$D_\mu\varphi \to [\partial_\mu + ieA_\mu + i(\partial_\mu\varepsilon)]e^{-i\varepsilon}\varphi = e^{-i\varepsilon}D_\mu\varphi. \tag{4.27}$$

In other words, the covariant derivative of φ transforms in the same way as φ itself, so that

$$\mathcal{L}_{KG} = (D_\mu\varphi)^*(D^\mu\varphi) - m^2\varphi^*\varphi \tag{4.28}$$

remains unchanged.

This is a profound result: we have found that the electromagnetic field is an essential requirement if the theory is to remain invariant under local phase transformations of a complex (i.e. charged) field. Furthermore the interaction between the fields must be of the form prescribed by the covariant derivative (4.26). Bearing in mind that in quantum mechanics the *canonical* 4-momentum is obtained from the wave function using the operator $i\partial^\mu$ (in units where $\hbar = 1$), we see that the covariant derivative operator D^μ represents the *mechanical* 4-momentum.

4.4 Electromagnetic Interaction

Expanding Eq. (4.28), we find

$$\mathcal{L}_{KG} = \partial_\mu\varphi^*\partial^\mu\varphi - m^2\varphi^*\varphi + ieA_\mu[(\partial^\mu\varphi^*)\varphi - \varphi^*(\partial^\mu\varphi)] + e^2A_\mu A^\mu\varphi^*\varphi. \tag{4.29}$$

The first two terms on the r.h.s. are those of the free-field Klein-Gordon equation. The third is the expected interaction term $eA_\mu J^\mu$ where J^μ is the free-field current (4.17). In addition, we now have a surprising extra term, quadratic in the electromagnetic potential, which is required to preserve gauge invariance.

Let us now apply Noether's theorem to deduce the conserved current associated with invariance of the combined charged scalar + electromagnetic field Lagrangian density

$$\mathcal{L} = \mathcal{L}_{em} + \mathcal{L}_{KG} = -\frac{1}{4}F_{\mu\nu}F^{\mu\nu} + (D_\mu\varphi)^*(D^\mu\varphi) - m^2\varphi^*\varphi, \tag{4.30}$$

under the infinitesimal local phase + gauge transformation

$$\varphi \to \varphi - ie\varepsilon\varphi, \quad A_\mu \to a_\mu + \partial_\mu\varepsilon. \tag{4.31}$$

We have

$$J^\mu \propto -ie\frac{\partial\mathcal{L}}{\partial(\partial_\mu\varphi)}\varepsilon\varphi + ie\frac{\partial\mathcal{L}}{\partial(\partial_\mu\varphi^*)}\varepsilon\varphi^* + \frac{\partial\mathcal{L}}{\partial(\partial_\mu A_\nu)}\partial_\nu\varepsilon. \tag{4.32}$$

The first two terms get contributions only from $\mathcal{L}_{KG}$, proportional to

$$J^\mu_{KG} = ie[\varphi^*(D^\mu\varphi) - (D^\mu\varphi)^*\varphi] = ie[\varphi^*(\partial^\mu\varphi) - (\partial^\mu\varphi)^*\varphi] - 2e^2A^\mu\varphi^*\varphi. \tag{4.33}$$

Thus the Klein-Gordon current is modified in the presence of the electromagnetic field, and the interaction of the extra piece gives rise to the final term in Eq. (4.29).

The third term in Eq. (4.32) gets a contribution only from $\mathcal{L}_{em}$:

$$J^\mu_{em} \propto -F^{\mu\nu}\partial_\nu\varepsilon = -\partial_\nu(F^{\mu\nu}\varepsilon) + (\partial_\nu F^{\mu\nu})\varepsilon. \tag{4.34}$$

As usual, we drop the first term on the r.h.s. since a total derivative cannot contribute to the charge as long as the fields vanish on the surface of the integration region. This leaves us with the current

$$J^{\mu}_{em} = \partial_{\nu} F^{\mu\nu}, \tag{4.35}$$

which is indeed conserved since

$$\partial_{\mu} J^{\mu}_{em} = \partial_{\mu}\partial_{\nu} F^{\mu\nu} = 0, \tag{4.36}$$

by the antisymmetry of the field strength tensor $F^{\mu\nu}$.

4.5 Stress-Energy (-Momentum) Tensor

If the symmetry involves a space-time transformation instead of (or in addition to) a redefinition of the fields at each space-time point, the situation is a little more complicated, because after the transformation the Lagrangian density is defined at the transformed point. Let us consider in particular a small space-time displacement, $x^{\mu} \to x^{\mu} + \varepsilon^{\mu}$. The corresponding field transformation is (always working to first order in ε)

$$\varphi(x^{\mu}) \to \tilde{\varphi}(x^{\mu}) = \varphi(x^{\mu} + \varepsilon^{\mu}) = \varphi + \varepsilon^{\mu}\partial_{\mu}\varphi = \varphi + \varepsilon_{\mu}\partial^{\mu}\varphi. \tag{4.37}$$

Provided the Lagrangian does not depend *explicitly* on the space-time coordinates, for this to be a symmetry transformation we require

$$\mathcal{L}(\tilde{\varphi}, \partial^{\mu}\tilde{\varphi}) = \mathcal{L}(x^{\mu} + \varepsilon^{\mu}) = \mathcal{L} + \varepsilon_{\mu}\partial^{\mu}\mathcal{L}. \tag{4.38}$$

Combining this condition with the expansion

$$\mathcal{L}(\tilde{\varphi}, \partial^{\mu}\tilde{\varphi}) = \mathcal{L}(\varphi, \partial^{\mu}\varphi) + \varepsilon_{\mu}\frac{\partial\mathcal{L}}{\partial\varphi}\partial^{\mu}\varphi + \varepsilon_{\mu}\frac{\partial\mathcal{L}}{\partial(\partial^{\nu}\varphi)}\partial^{\mu}\partial^{\nu}\varphi, \tag{4.39}$$

and recalling that ε_{μ} is an arbitrary constant, we obtain

$$\frac{\partial\mathcal{L}}{\partial\varphi}\partial^{\mu}\varphi + \frac{\partial\mathcal{L}}{\partial(\partial^{\nu}\varphi)}\partial^{\mu}\partial^{\nu}\varphi = \partial^{\mu}\mathcal{L}. \tag{4.40}$$

As in the derivation of the Noether current, we may now use the equation of motion to write this as

$$\partial^{\nu}\left(\frac{\partial\mathcal{L}}{\partial(\partial^{\nu}\varphi)}\partial^{\mu}\varphi\right) = \partial^{\mu}\mathcal{L}, \tag{4.41}$$

or in other words

$$\partial^{\nu}\left(\frac{\partial\mathcal{L}}{\partial(\partial^{\nu}\varphi)}\partial^{\mu}\varphi - \delta^{\mu}_{\nu}\mathcal{L}\right) = 0. \tag{4.42}$$

Relabelling and rearranging indices, we see that this implies that the **stress-energy tensor**,

$$T^{\mu\nu} = \frac{\partial\mathcal{L}}{\partial(\partial_{\mu}\varphi)}\partial^{\nu}\varphi - g^{\mu\nu}\mathcal{L}, \tag{4.43}$$

(sometimes called the energy-momentum tensor) is conserved:

$$\partial_{\mu} T^{\mu\nu} = 0. \tag{4.44}$$

As in the case of the Noether current, for multi-component fields we have simply to add the contributions of the components:

$$T^{\mu\nu} = \sum_{j} \frac{\partial\mathcal{L}}{\partial(\partial_{\mu}\varphi_j)}\partial^{\nu}\varphi_j - g^{\mu\nu}\mathcal{L}. \tag{4.45}$$

4.5.1 Longitudinal waves in 1D

Although we have used relativistic notation, these results are not limited to covariant systems, as long as the Lagrangian density is invariant under translations in space and time. For longitudinal waves on an elastic rod, for example, we saw that

$$\mathcal{L} = \frac{1}{2}\rho(\dot{\varphi})^2 - \frac{1}{2}\kappa(\varphi')^2, \tag{4.46}$$

and therefore

$$\begin{aligned} T_{tt} &= \rho(\dot{\varphi})^2 - \mathcal{L} = \mathcal{H}, & T_{tx} &= -\rho\dot{\varphi}\varphi', \\ T_{xx} &= \kappa(\varphi')^2 + \mathcal{L} = \mathcal{H}, & T_{xt} &= -\kappa\dot{\varphi}\varphi'. \end{aligned} \tag{4.47}$$

As expected, T_{tt} is the Hamiltonian density, i.e. the wave energy per unit length in the rod. Furthermore from Eq. (4.44)

$$\frac{\partial T_{tt}}{\partial t} = -\frac{\partial T_{xt}}{\partial x}, \tag{4.48}$$

as can easily be verified using the equation of motion, so that $T_{xt} = -\kappa\dot{\varphi}\varphi'$ must represent the flow of wave energy along the rod. Similarly

$$\frac{\partial T_{tx}}{\partial t} = -\frac{\partial T_{xx}}{\partial x}, \tag{4.49}$$

where T_{tx} is the momentum density in the wave and T_{xx} is the associated flow of momentum (which in this case coincides again with the energy (Hamiltonian) of the system, as per (4.47)).

4.5.2 Relativistic Scalar Field

In the case of a relativistic scalar field, we saw that the field must satisfy the Klein-Gordon equation, with Lagrangian density (3.30):

$$\mathcal{L} = \frac{1}{2}(\partial^\mu\varphi)(\partial_\mu\varphi) - \frac{1}{2}m^2\varphi^2. \tag{4.50}$$

Thus the stress-energy tensor is

$$T^{\mu\nu} = (\partial^\mu\varphi)(\partial^\nu\varphi) - g^{\mu\nu}\mathcal{L}. \tag{4.51}$$

4.5.3 Electromagnetic Field

For the free electromagnetic field (in units where $\mu_0 = \epsilon_0 = c = 1$) we have

$$\mathcal{L} = -\frac{1}{4}F_{\alpha\beta}F^{\alpha\beta} = -\frac{1}{4}g^{\alpha\gamma}g^{\beta\delta}(\partial_\alpha A_\beta - \partial_\beta A_\alpha)(\partial_\gamma A_\delta - \partial_\delta A_\gamma), \tag{4.52}$$

and the stress-energy tensor is

$$\begin{aligned} T^{\mu\nu} &= \frac{\partial\mathcal{L}}{\partial(\partial_\mu A_\lambda)}\partial^\nu A_\lambda - g^{\mu\nu}\mathcal{L} \\ &= -F^{\mu\lambda}\partial^\nu A_\lambda + \frac{1}{4}g^{\mu\nu}F_{\alpha\beta}F^{\alpha\beta} \\ &= -F^\mu_\lambda\partial^\nu A^\lambda + \frac{1}{4}g^{\mu\nu}F_{\alpha\beta}F^{\alpha\beta}. \end{aligned} \tag{4.53}$$

While this is indeed a conserved tensor, it is not in a convenient form since it is not gaugeinvariant and cannot be expressed in terms of the field strengths $\mathbf{E}$ and $\mathbf{B}$. Notice, however, that we are free to redefine $T^{\mu\nu}$ by adding any tensor of the form $\partial_\lambda \Omega^{\lambda\mu\nu}$ where $\Omega^{\lambda\mu\nu}$ is antisymmetric with respect to the indices λ and μ, for then $\partial_\mu\partial_\lambda\Omega^{\lambda\mu\nu} = 0$ (this is true for any stress-energy tensor, not only in the case of an electromagnetic field). Let us choose

$$\Omega^{\lambda\mu\nu} = -F^{\lambda\mu}A^\nu. \tag{4.54}$$

so that the added terms are

$$\partial_\lambda \Omega^{\lambda\mu\nu} = -(\partial_\lambda F^{\lambda\mu})A^\nu - F^{\lambda\mu}\partial_\lambda A^\nu. \tag{4.55}$$

By virtue of the free-field Maxwell equations (3.79), the first term on the r.h.s. vanishes (in the absence of sources), and therefore

$$\partial_\lambda \Omega^{\lambda\mu\nu} = -F^{\lambda\mu}\partial_\lambda A^\nu = F^{\mu\lambda}\partial_\lambda A^\nu = F^\mu{}_\lambda\, \partial^\lambda A^\nu. \tag{4.56}$$

Our redefined stress-energy tensor is thus

$$T^{\mu\nu} = -F^\mu{}_\lambda F^{\nu\lambda} + \frac{1}{4} g^{\mu\nu} F_{\alpha\beta}F^{\alpha\beta}, \tag{4.57}$$

which is now expressed in terms of the field strengths and therefore gauge invariant. Notice that it is also now a symmetric tensor, which means for example that $T^{01} = T^{10}$, i.e. the density of the x-component of the field momentum is equal to the flow of energy in the x-direction. In terms of the field strengths, we have explicitly

$$\mathcal{L} = \frac{1}{2}\Big(\mathbf{E}^2 - \mathbf{B}^2\Big), \quad T^{00} = \mathcal{H} = \frac{1}{2}\Big(\mathbf{E}^2 + \mathbf{B}^2\Big), \quad T^{0j} = (\mathbf{E}\times\mathbf{B})_j. \tag{4.58}$$

You may recognise that the term on the right is none other than the j-component of the Poynting vector, which is indeed the directional energy flux density of an electromagnetic field.

4.5.4 General Relativity

In general relativity, the element of space-time that is invariant under general coordinate transformations is $\mathrm{d}^4x\,\sqrt{-g}$ where g is the determinant of the metric tensor, $g = \det(g_{\mu\nu})$, which is of course -1 for the Minkowski metric (2.62). The invariant action integral therefore becomes

$$S = \int \mathrm{d}^4x\,\sqrt{-g}\mathcal{L}. \tag{4.59}$$

There is then a very general and powerful way of defining the stress-energy tensor, which is to say that it measures the response of the action to small changes in the metric, according to the equation

$$\delta S = \frac{1}{2}\int \mathrm{d}^4x\,\sqrt{-g}T_{\mu\nu}\delta g^{\mu\nu}, \tag{4.60}$$

that is,

$$T_{\mu\nu} = \frac{2}{\sqrt{-g}}\frac{\partial(\sqrt{-g}\mathcal{L})}{\partial g^{\mu\nu}} = 2\frac{\partial\mathcal{L}}{\partial g^{\mu\nu}} + \frac{1}{g}\frac{\partial g}{\partial g^{\mu\nu}}\mathcal{L}. \tag{4.61}$$

Now from the properties of determinants and the inverse matrix,

$$\frac{\partial(\det M)}{\partial M_{jk}} = \det M (M^{-1})_{kj}, \tag{4.62}$$

and (even in general relativity)

$$g_{\mu\lambda} g^{\nu\lambda} = \delta^{\nu}_{\mu}, \tag{4.63}$$

so $(g^{-1})^{\nu\mu} = g^{\mu\nu}$ and

$$\frac{\partial g}{\partial g_{\mu\nu}} = g g^{\mu\nu}. \tag{4.64}$$

This is almost what we need: differentiating (4.63) gives $g_{\mu\lambda}\, \mathrm{d}g^{\nu\lambda} = -\,\mathrm{d}g_{\mu\lambda}\, g^{\nu\lambda}$, so $\mathrm{d}g_{\mu\nu} = -g_{\mu\lambda} g_{\sigma\nu}\, \mathrm{d}g^{\sigma\lambda}$ and

$$\frac{\partial g}{\partial g^{\mu\nu}} = -g g_{\mu\nu}. \tag{4.65}$$

Thus we finally obtain for the stress-energy tensor the general expression

$$T_{\mu\nu} = 2\frac{\partial \mathcal{L}}{\partial g^{\mu\nu}} - g_{\mu\nu}\mathcal{L}. \tag{4.66}$$

You can check that (4.66) agrees with the results we obtained earlier for the Klein-Gordon and electromagnetic fields. Notice that this tensor is manifestly symmetric (since $g_{\mu\nu}$ is) and we automatically obtain the symmetric, gauge-invariant form (4.57) in the electromagnetic case.

4.6 Angular Momentum and Spin

Having found that the stress-energy tensor $T^{\mu\nu}$ is conserved and (properly defined) symmetric, we can construct a conserved tensor of higher rank as follows:

$$M^{\lambda\mu\nu} = x^{\mu} T^{\lambda\nu} - x^{\nu} T^{\lambda\mu}, \tag{4.67}$$

for then,

$$\partial_{\lambda} M^{\lambda\mu\nu} = T^{\mu\nu} - T^{\nu\mu} = 0, \tag{4.68}$$

since $T^{\mu\nu}$ is symmetric. Recalling that T^{0j} is the density of the j^{th} component of momentum, we see that for example $M^{012} = xT^{02} - yT^{01}$ is the density of the z-component of angular momentum, and so we define the *total angular momentum tensor* of the field as

$$J^{\mu\nu} = \int \mathrm{d}^3\mathbf{r}\, M^{0\mu\nu}. \tag{4.69}$$

Let us open a parenthesis here to remark how we have arrived at a conserved angular momentum. At the beginning of Section 4.5 we introduced the conserved stress-energy tensor as a consequence of invariance to small space-time displacements. In general, this symmetry alone does not warrant conservation of *angular* momentum. However, we considered systems that have a larger symmetry: invariance with respect to general coordinate transformations. These include rotations and thus lead to conservation of the total angular momentum. In this section we see that this additional conservation is

directly related to whether the stress-energy tensor is symmetric or not in (some of) its space-time indices.

The components of the more familiar total angular momentum vector $\mathbf{J}$ are then given by

$$J_i = \frac{1}{2}\varepsilon_{ijk}J^{jk}. \tag{4.70}$$

The other non-zero components of $J^{\mu\nu}$ are of the form

$$J^{0j} = -J^{j0} = \int \mathrm{d}^3\mathbf{r}\, M^{00j} = t\int \mathrm{d}^3\mathbf{r}\, T^{0j} - \int \mathrm{d}^3\mathbf{r}\, x^j T^{00} = tP_j - R_j E, \tag{4.71}$$

where $\mathbf{P}$ is the total momentum of the field, E the total energy, and $\mathbf{R}$ the position of the centre-of-energy. Thus the conservation of this quantity implies that

$$\mathbf{R} = \mathbf{V}t + \text{const.}, \tag{4.72}$$

where $\mathbf{V} = \mathbf{P}/E$ is the velocity of the centre-of-energy, i.e. the velocity of the zero-momentum frame (in units where $c = 1$). This is just Newton's first law: the centre-of-energy of an isolated system moves with constant velocity.

Since in general the centre-of-energy is moving, the total angular momentum includes both "orbital" and "intrinsic" parts, where the intrinsic or *spin* angular momentum is defined in the zero-momentum frame. We can make a covariant definition of the spin by using the 4-velocity $U^\mu P^\mu/\sqrt{P_\nu P^\nu} = \gamma(1, \mathbf{V})$, where $\gamma = 1/\sqrt{1-V^2}$. Then we define the *spin 4-vector* as

$$S^\mu = -\frac{1}{2}\varepsilon^{\mu\nu\alpha\beta}U_\nu J_{\alpha\beta}, \tag{4.73}$$

where $\varepsilon^{\mu\nu\alpha\beta}$ is the totally antisymmetric Levi-Civita tensor ($\varepsilon = +1$ for any even permutation of indices 0123, -1 for any odd permutation, 0 otherwise). Then in the zero-momentum frame $U_\nu = (1, \mathbf{0})$, $S^0 = 0$ and

$$S^i = -\frac{1}{2}\varepsilon^{i0jk}J_{jk} = J^i. \tag{4.74}$$

Notice that S^μ is always orthogonal to the 4-velocity, $S^\mu U_\mu = 0$, so in fact the spin only has 3 independent components in any frame, whereas $J^{\mu\nu}$ has the extra components (4.71), which are mixed with those of $\mathbf{J}$ in different frames. There is no covariant way of separating the total angular momentum into orbital and spin contributions. J is a 4-tensor and S is a 4-vector: to take their difference "$L = J - S$" does not make sense, any more than subtracting apples from oranges.

4.7 Quantum Fields

Although this is a course on classical field theory, it is worth making a short excursion into the quantum mechanics of fields, which in fact clarifies many of their properties, especially in the relativistic case. The transition from classical to quantum fields is through a procedure called 'second quantisation'.

First quantisation was the procedure of replacing the classical dynamical variables q and p by quantum operators $\hat{q}$ and $\hat{p}$ such that

$$[\hat{q}, \hat{p}] = i \qquad (\hbar = 1). \tag{4.75}$$

Second quantisation means replacing the field variable $\varphi(x,t)$ and its conjugate momentum density $\pi(x,t)$ by operators such that

$$[\hat{\varphi}(x,t), \hat{\pi}(x',t)] = i\delta(x - x'). \tag{4.76}$$

N.B.: x and x' are not dynamical variables but labels for the field values at different points. Compare (and contrast)

$$[\hat{q}_j, \hat{p}_k] = i\delta_{jk} \qquad (j,k = x,y,z). \tag{4.77}$$

The field (wavefunction) φ satisfying the Klein-Gordon equation is replaced by a *field operator* $\hat{\varphi}$, satisfying the same equation. The Fourier representation of a real field becomes

$$\hat{\varphi}(x,t) = \int \mathrm{d}k\, N(k)\Big[\hat{a}(k)e^{i(kx-\omega t)} + \hat{a}^\dagger(k)e^{-i(kx-\omega t)}\Big]. \tag{4.78}$$

Note that $\hat{\varphi}$ is hermitian but the Fourier conjugate operator $\hat{a}$ is not. Keeping track of the order of operators, the Hamiltonian operator is

$$\hat{H} = \int \mathrm{d}k\, N(k)\frac{1}{2}\omega(k)\Big[\hat{a}(k)\hat{a}^\dagger(k) + \hat{a}^\dagger(k)\hat{a}(k)\Big]. \tag{4.79}$$

Comparing this with the simple harmonic oscillator,

$$\hat{H}_{\mathrm{SHO}} = \frac{1}{2}\omega\Big(\hat{a}\hat{a}^\dagger + \hat{a}^\dagger\hat{a}\Big), \tag{4.80}$$

we see that $\hat{a}^\dagger(k)$ and $\hat{a}(k)$ must be the ladder operators for the mode of wave number k. They add/remove one quantum of excitation of the mode. These quanta are the particles corresponding to that field

$$\Longrightarrow \quad \hat{a}^\dagger(k) = \text{the } \textit{creation} \text{ operator}, \quad \hat{a}(k) = \text{the } \textit{annihilation} \text{ operator} \tag{4.81}$$

for Klein-Gordon particles.

The ladder operators of the simple harmonic oscillator satisfy

$$\Big[\hat{a}, \hat{a}^\dagger\Big] = 1. \tag{4.82}$$

The analogous commutation relation for the creation and annihilation operators is

$$\begin{aligned} &N(k)\Big[\hat{a}(k), \hat{a}^\dagger(k')\Big] = \delta(k - k') \\ &\Longrightarrow \ \Big[\hat{a}(k), \hat{a}^\dagger(k')\Big] = 2\pi \cdot 2\omega(k)\delta(k - k'), \end{aligned} \tag{4.83}$$

or in 3 spatial dimensions

$$\Big[\hat{a}(\mathbf{k}), \hat{a}^\dagger(\mathbf{k}')\Big] = (2\pi)^3 \cdot 2\omega(\mathbf{k})\delta^3(\mathbf{k} - \mathbf{k}'). \tag{4.84}$$

On the other hand

$$[\hat{a}(\mathbf{k}), \hat{a}(\mathbf{k}')] = \left[\hat{a}^\dagger(\mathbf{k}), \hat{a}^\dagger(\mathbf{k}')\right] = 0. \tag{4.85}$$

The commutators of the creation and annihilation operators correspond to the field commutation relation

$$\begin{aligned}[\hat{\varphi}(\mathbf{r}, t), \hat{\pi}(\mathbf{r}', t)] &= \int \mathrm{d}^3\mathbf{k}\, \mathrm{d}^3\mathbf{k}'\, N(\mathbf{k}) N(\mathbf{k}') [-i\omega(\mathbf{k}')] \\ &\quad \times \left[\hat{a}(\mathbf{k}) e^{-ik\cdot x} + \hat{a}^\dagger(\mathbf{k}) e^{ik\cdot x}, \hat{a}(\mathbf{k}') e^{-ik'\cdot x'} - \hat{a}^\dagger(\mathbf{k}') e^{ik'\cdot x'}\right] \\ &= i \int \mathrm{d}^3\mathbf{k}\, N(\mathbf{k}) \omega(\mathbf{k}) \left[e^{-ik\cdot(x-x')} + e^{ik\cdot(x-x')}\right], \end{aligned} \tag{4.86}$$

where $x^\mu = (ct, \mathbf{r})$ and $x'^\mu = (ct, \mathbf{r}')$. Hence

$$[\hat{\varphi}(\mathbf{r}, t), \hat{\pi}(\mathbf{r}', t)] = i\delta^3(\mathbf{r} - \mathbf{r}'), \tag{4.87}$$

as expected. On the other hand

$$[\hat{\varphi}(\mathbf{r}, t), \hat{\varphi}(\mathbf{r}', t)] = [\hat{\pi}(\mathbf{r}, t), \hat{\pi}(\mathbf{r}', t)] = 0. \tag{4.88}$$

The fact that the field operator has positive- and negative-frequency parts now appears quite natural:

- The *positive* frequency part $\hat{a}(\mathbf{k}) e^{i(\mathbf{k}\cdot\mathbf{r} - \omega t)}$ *annihilates* particles;
- The *negative* frequency part $\hat{a}^\dagger(\mathbf{k}) e^{-i(\mathbf{k}\cdot\mathbf{r} - \omega t)}$ *creates* particles;

and $\pm\hbar\omega$ is the energy released/absorbed in the annihilation/creation process.

The hermitian field describes particles that are identical to their antiparticles, e.g. π^0 mesons. For a complex (non-hermitian) field, the negative-frequency part of $\hat{\varphi}$ *creates antiparticles*. To see this, consider the second-quantised version of Eq. (4.22) for a complex field $\hat{\varphi}$:

$$\hat{Q} = \int \mathrm{d}^3\mathbf{k}\, N(\mathbf{k}) \left[\hat{a}^\dagger(\mathbf{k}) \hat{a}(\mathbf{k}) - \hat{b}^\dagger(\mathbf{k}) \hat{b}(\mathbf{k})\right]. \tag{4.89}$$

Comparing with the energy

$$\hat{H} = \int \mathrm{d}^3\mathbf{k}\, N(\mathbf{k}) \omega(\mathbf{k}) \left[\hat{a}^\dagger(\mathbf{k}) \hat{a}(\mathbf{k}) + \hat{b}^\dagger(\mathbf{k}) \hat{b}(\mathbf{k})\right], \tag{4.90}$$

we see that the particles created by $\hat{a}^\dagger$ and $\hat{b}^\dagger$ have the same energy $\hbar\omega$ but *opposite charge*: for example, they could be π^+ and π^- mesons.

To summarise, in quantum field theory:

- The object that satisfies the Klein-Gordon equation is the field operator $\hat{\varphi}$;
- The Fourier decomposition of $\hat{\varphi}$ has a *positive frequency* part that *annihilates a particle* (with energy $\hbar\omega$ and charge $+1$) AND a *negative frequency* part that *creates an antiparticle* (with energy $\hbar\omega$ and charge -1);
- Similarly, $\hat{\varphi}^\dagger$ creates a particle or annihilates an antiparticle.

Chapter 5

Broken Symmetry

We have seen that symmetries can have profound implications (e.g., conserved currents), but sometime the breaking of symmetry can be even more interesting. We introduce here the important phenomenon of *spontaneous* symmetry breaking, in the simple context of the scalar Klein-Gordon field. We consider only the classical case, but all the features of interest remain valid after second quantisation.

5.1 Self-Interacting Scalar Field

Let us consider the effect of adding terms of higher order in the field φ to the Klein-Gordon Lagrangian density (3.69). The simplest addition that preserves the global phase symmetry is a quartic term $-\frac{1}{2}\lambda(\varphi^*\varphi)^2$:

$$\mathcal{L} = (\partial^\mu\varphi^*)(\partial_\mu\varphi) - m^2\varphi^*\varphi - \frac{1}{2}\lambda(\varphi^*\varphi)^2. \tag{5.1}$$

As was argued earlier for the quadratic term $-m^2\varphi^*\varphi$, the coefficient λ must be positive in order for the Hamiltonian to be positive-definite, otherwise no state of lowest energy will exist.

Notice that λ is a dimensionless quantity: this is easy to see in natural units, since then $\mathcal{L}$ and $(\varphi^*\varphi)^2$ both have dimensions $[M]^4$. Any higher powers, $(\varphi^*\varphi)^p$ with $p > 2$, would have coefficients with dimensions of inverse powers of mass, $[M]^{4-2p}$. One can argue on rather general grounds that such terms should be negligible since the relevant mass scale should be large.

The equation for the conjugate momentum density, $\pi = \partial\varphi^*/\partial t$, remains unchanged and the Hamiltonian density is

$$\mathcal{H} = \pi^*\pi + \boldsymbol{\nabla}\varphi^* \cdot \boldsymbol{\nabla}\varphi + V(\varphi), \tag{5.2}$$

where the 'potential' is

$$V(\varphi) = m^2\varphi^*\varphi + \frac{1}{2}\lambda(\varphi^*\varphi)^2. \tag{5.3}$$

The equation of motion becomes

$$\partial^\mu\partial_\mu\varphi + m^2\varphi + \lambda(\varphi^*\varphi)\varphi = 0. \tag{5.4}$$

We can think of the extra term as a self-interaction of the field, with strength λ.

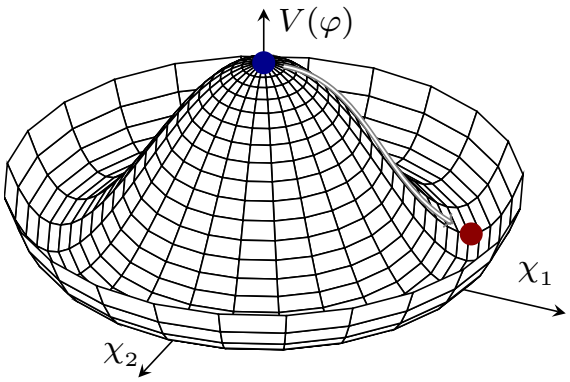

Fig. 5.1: The form of the 'potential' $V(\varphi)$ that leads to spontaneous symmetry breaking.

5.2 Spontaneously Broken Global Symmetry

The Hamiltonian density (5.2) with the potential (5.3) implies that the state of the field with minimum energy is that in which $\varphi = 0$ everywhere (assuming that the coefficient m^2 of the quadratic term is non-negative). Note, however, that in the presence of the quartic term in the potential our previous argument for the positive sign of the quadratic term (see Section 3.3) is no longer valid: the Hamiltonian is always bounded from below as long as $\lambda > 0$. Let us therefore study the effect of a negative quadratic term in the potential, i.e.

$$V(\varphi) = -m^2\varphi^*\varphi + \frac{1}{2}\lambda(\varphi^*\varphi)^2. \tag{5.5}$$

The state of minimum energy will now be one in which φ has a constant value φ_0 such that $V(\varphi_0)$ is a minimum, i.e.

$$\varphi_0^*\varphi_0 = \frac{m^2}{\lambda}, \tag{5.6}$$

which describes a circle in the complex φ plane,

$$\varphi_0 = \frac{m}{\sqrt{\lambda}}e^{i\theta}, \tag{5.7}$$

where θ is arbitrary.

Thus the system does not have a unique state of minimum energy but an infinite number of equivalent ones corresponding to different values of θ: it is said to be *degenerate*. However, if we take any particular example of the system and reduce its energy somehow to the minimum value, it will be in a state with a particular value of θ. The situation is like that of a thin rod initially balanced vertically on its tip on a horizontal plane: when it falls under gravity, it will lie at a particular angle on the plane, although all angles have equal energy. The dynamics and the initial state are symmetrical with respect to rotations about the vertical axis, but the final minimum-energy state is not: the rotational symmetry has been *spontaneously broken*.

Similarly, in the presence of the quartic interaction, the Klein-Gordon field will undergo spontaneous symmetry breaking by choosing some particular minimum-energy state, with a particular global value of θ. And since the dynamics has phase symmetry we may as well choose to label that state as $\theta = 0$ (like measuring angles with respect to the fallen

rod). Thus we define $\varphi_0 = m/\sqrt{\lambda}$ and measure variations of the field with respect to this 'ground-state' value: $\varphi = \varphi_0 + \chi$ (for instance, if we are interested in fluctuations of the system about the symmetry broken ground state φ_0). In terms of the 'dynamical' field χ, the potential is

$$\begin{aligned} V &= V(\varphi_0) + \frac{1}{2}\lambda[\varphi_0(\chi^* + \chi) + \chi^*\chi]^2 \\ &= V(\varphi_0) + \frac{1}{2}m^2(\chi^* + \chi)^2 + \mathcal{O}(\chi^3) \end{aligned} \tag{5.8}$$

(where we have used the fact that $\lambda\varphi_0^2 = m^2$ to cancel a lot of terms). Resolving χ into its real and imaginary parts as in Eq. (3.61):

$$\chi = \frac{1}{\sqrt{2}}(\chi_1 + i\chi_2), \tag{5.9}$$

where χ_1 and χ_2 are real, we have

$$V = V(\varphi_0) + m^2\chi_1^2 + \mathcal{O}(\chi^3), \tag{5.10}$$

and the Lagrangian and Hamiltonian reduce to, respectively:

$$\mathcal{L} = \frac{1}{2}(\partial^\mu\chi_1)(\partial_\mu\chi_1) + \frac{1}{2}(\partial^\mu\chi_2)(\partial_\mu\chi_2) - V(\varphi_0) - m^2\chi_1^2 + \mathcal{O}(\chi^3) \tag{5.11}$$

$$\begin{aligned} \mathcal{H} = &\frac{1}{2}\left(\frac{\partial\chi_1}{\partial t}\right)^2 + \frac{1}{2}\boldsymbol{\nabla}\chi_1 \cdot \boldsymbol{\nabla}\chi_1 + m^2\chi_1^2 \\ &+ \frac{1}{2}\left(\frac{\partial\chi_2}{\partial t}\right)^2 + \frac{1}{2}\boldsymbol{\nabla}\chi_2 \cdot \boldsymbol{\nabla}\chi_2 + V(\varphi_0) + \mathcal{O}(\chi^3), \end{aligned} \tag{5.12}$$

where we immediately recognise the separate contributions pertaining to the fields χ_1 and χ_2.

Equation (5.10) displays many interesting features:

1. The phase symmetry breaking is now explicit: there is a quadratic term for the real part of χ but not for the imaginary part;
2. The quadratic term for the real part φ_1 is positive even though we started off with a negative quadratic term for φ.
3. Comparing with the original Klein-Gordon equation (3.30), we see that the quadratic term corresponds to the dispersion relation

   $$\omega = \sqrt{k^2 + 2m^2} \tag{5.13}$$

   for the field χ_1. This means that, after second-quantisation, the quanta of the field will be particles of mass (in natural units) $\sqrt{2}m$;
4. On the other hand the field χ_2 has no quadratic term and therefore its dispersion relation is $\omega = k$, i.e. its quanta have zero mass, like those of the electromagnetic field (photons), except that their spin is zero instead of one.

This last point is an example of *Goldstone's theorem*: for every spontaneously broken (global) continuous symmetry there is a field with massless quanta, which is therefore called a Goldstone field.

5.3 Spontaneously Broken Local Symmetry

Recall that the symmetry of the Klein-Gordon Lagrangian with respect to global (space-time independent) phase changes can be promoted to local (space-time dependent) phase symmetry by introducing a vector field A^μ that undergoes a compensating gauge transformation. The full Lagrangian density then takes the form

$$\mathcal{L} = -\frac{1}{4}F_{\mu\nu}F^{\mu\nu} + (D_\mu\varphi)^*(D^\mu\varphi) - V(\varphi), \tag{5.14}$$

where $D_\mu = \partial_\mu + ieA_\mu$. As in the previous subsection, the presence of negative quadratic and positive quartic terms in V will trigger spontaneous symmetry breaking and a non-zero value of φ satisfying Eq. (5.6) in the state of minimum energy. However, in such a state (i.e., $\varphi = \varphi_0$) we now obtain a non-zero contribution to $\mathcal{L}$ from the second term on the r.h.s., namely

$$(ie\varphi_0 A_\mu)^*(ie\varphi_0 A^\mu) = \frac{e^2m^2}{\lambda}A_\mu A^\mu, \tag{5.15}$$

and the corresponding equation of motion for the field A_μ (in Lorenz gauge, $\partial_\mu A^\mu = 0$) is

$$\partial_\nu\partial^\nu A_\mu + 2\frac{e^2m^2}{\lambda}A_\mu = 0. \tag{5.16}$$

This means that the dispersion relation for the vector field has become

$$\omega = \sqrt{k^2 + 2e^2m^2/\lambda}, \tag{5.17}$$

and correspondingly the quanta of the vector field have acquired a non-zero mass equal to $em\sqrt{2/\lambda}$. In the following section we shall see in detail how this generation of mass has come to pass, through a phenomenon known as the *Higgs mechanism*.

5.4 Higgs Mechanism

Let us examine what happens to the dynamical part of the scalar field when the local phase symmetry is spontaneously broken. As in the case of global symmetry breaking, we write

$$\varphi = \varphi_0 + \chi = \varphi_0 + \frac{1}{\sqrt{2}}(\chi_1 + i\chi_2). \tag{5.18}$$

When χ is non-zero, the covariant derivative of φ becomes

$$D_\mu\varphi = \frac{1}{\sqrt{2}}(\partial_\mu\chi_1 + i\partial_\mu\chi_2) + ie\varphi_0 A_\mu + \cdots, \tag{5.19}$$

where the dots represent terms of higher order in the fields. We see that the term involving χ_2 can be removed by a redefinition of the vector field

$$A_\mu \to A_\mu - \frac{1}{\sqrt{2}e\varphi_0}\partial_\mu\chi_2, \tag{5.20}$$

which is just a gauge transformation, so it leaves the field strength tensor $F_{\mu\nu}$ unchanged. The Lagrangian density then takes the form

$$\begin{aligned}\mathcal{L} &= -\frac{1}{4}F_{\mu\nu}F^{\mu\nu} + e^2\varphi_0^2 A_\mu A^\mu + \frac{1}{2}(\partial_\mu\chi_1)(\partial^\mu\chi_1) - V(\varphi) + \cdots \\ &= -\frac{1}{4}F_{\mu\nu}F^{\mu\nu} + \frac{e^2m^2}{\lambda}A_\mu A^\mu + \frac{1}{2}(\partial_\mu\chi_1)(\partial^\mu\chi_1) - m^2\chi_1^2 - V(\varphi_0) + \cdots . \end{aligned} \tag{5.21}$$

As we saw before, there is now a term quadratic in the vector field, which corresponds to its quanta having a mass, and a similar term for the dynamical scalar field χ_1. However, unlike the case of the broken *global* phase symmetry, there are no terms involving the field χ_2: it has been absorbed in a redefinition of the vector field. In more colourful terms, the vector field has *eaten* the Goldstone field and thereby acquired a mass. This is called the *Higgs mechanism*.

Another way to see that the field χ_2 can be removed by a gauge transformation is to recall that such a transformation is equivalent to a change of phase of the scalar field. Since χ_2 is the imaginary part of the field φ, it can be removed by a phase change

$$\varphi \to e^{-i\theta} \quad \text{where} \quad \theta = \sin^{-1}(\chi_2/|\varphi|), \tag{5.22}$$

which makes φ real everywhere. Local phase/gauge symmetry means we are allowed to make a different phase change at every space-time point, so χ_2 can always be removed in this way. In the absence of a vector field, on the other hand, we can only make a constant global phase change, so χ_2 cannot be removed and remains a physical field.

The Higgs mechanism can also be applied more generally when the Lagrangian density of a system has several local gauge symmetries, some of which are broken spontaneously by nonzero values of scalar fields in the state of minimum energy. For each gauge symmetry there is a vector field whose quanta are massless if the symmetry is unbroken but massive if it is broken. The masses are acquired by 'eating' the Goldstone components of the scalar fields, which would otherwise have massless quanta themselves. The remaining, uneaten components of the scalar fields have quanta that should be observable as massive *Higgs bosons*.

In the Standard Model of particle physics, the electromagnetic and weak nuclear interactions are described by a unified theory with four distinct gauge symmetries, three of which are broken spontaneously by components of a pair of complex scalar fields. Thus three of the four associated vector fields have massive quanta (the W^+, W^- and Z^0 bosons) while one remains massless (the photon). Correspondingly, three of the four (real and imaginary) components of the scalar fields are eaten and one physical scalar Higgs boson remains. In the Standard Model, the Higgs field also couples to the fundamental fermions (i.e. the quarks and leptons), and through these interactions the fermions also acquire mass (see Figure 5.2).

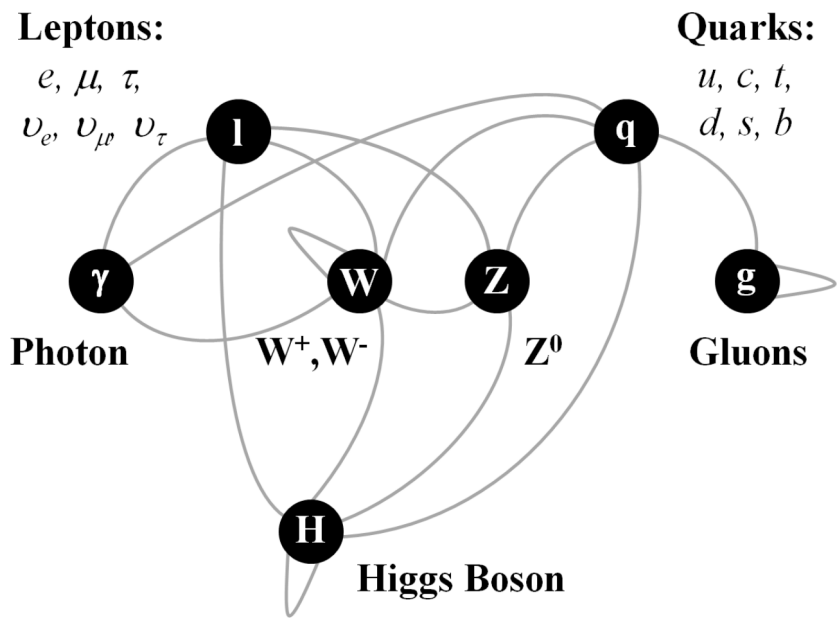

Fig. 5.2: Summary of interactions between particles described by the Standard Model.

Chapter 6

Dirac Field [*not examinable*]

You may have already encountered the relativistic wave equation for the electron, namely the so-called Dirac equation

$$i\hbar\frac{\partial\psi}{\partial t} = -i\hbar c\,\boldsymbol{\alpha}\cdot\boldsymbol{\nabla}\psi + \beta mc^2\psi, \tag{6.1}$$

where ψ is a 4-component wave function called a *Dirac spinor* and α_j, β are 4×4 hermitian *Dirac matrices* with the properties

$$\alpha_j^2 + \beta^2 = 1, \quad \alpha_j\beta + \beta\alpha_j = \alpha_j\alpha_k + \alpha_k\alpha_j = 0 \quad (i,j=1,2,3; j\neq k). \tag{6.2}$$

To make the covariant form of the Dirac equation more apparent, we multiply through by β and rearrange terms to give

$$i\hbar(\beta\partial_0\psi + c\beta\alpha_j\partial_j\psi) = mc^2\psi. \tag{6.3}$$

Defining

$$\gamma^0 = \beta, \quad \gamma^j = \beta\alpha_j, \tag{6.4}$$

and dividing by the speed of light c, we can write this as

$$i\hbar\gamma^\mu\partial_\mu\psi = mc\psi, \tag{6.5}$$

where one needs to recall that $\partial_0\ \partial/\partial(ct)$. In natural units:

$$(i\gamma^\mu\partial_\mu - m)\psi = 0. \tag{6.6}$$

From the properties of the α_j and β matrices we find (check it!) that

$$\{\gamma^\mu,\gamma^\nu\} = \gamma^\mu\gamma^\nu + \gamma^\nu\gamma^\mu = 2g^{\mu\nu}I_4, \tag{6.7}$$

where the curly brackets $\{\,,\,\}$ denote the so called anti-commutator, and ${}_I4$ is the 4×4 identity matrix. Whereas the notation may already look covariant, it is important to appreciate that γ^μ is NOT a 4-vector like x^μ or ∂_μ: it is a set of 4 4×4 matrices, which do not transform under Lorentz transformations.

In the so-called standard representation, the γ matrices take the form

$$\gamma^0 = \begin{pmatrix} I_2 & 0 \\ 0 & -I_2 \end{pmatrix}, \quad \gamma^i = \begin{pmatrix} 0 & \sigma_i \\ -\sigma_i & 0 \end{pmatrix}, \tag{6.8}$$

where I_2 is the 2×2 identity matrix and σ_i are Pauli matrices.

To make a 4-vector, we have to sandwich γ^μ between some spinors. Recall that the probability density associated with the Dirac spinor ψ is

$$\rho = \psi^\dagger\psi, \tag{6.9}$$

and the probability current is

$$\mathbf{J} = c\psi^\dagger \boldsymbol{\alpha}\psi. \tag{6.10}$$

Introducing the notation

$$\overline{\psi} = \psi^\dagger\beta = \psi^\dagger\gamma^0, \tag{6.11}$$

we have

$$\rho = \overline{\psi}\gamma^0\psi, \quad J_j = c\overline{\psi}\gamma^j\psi. \tag{6.12}$$

However, we know that the density and current together form a 4-vector $J^\mu = (c\rho, \mathbf{J})$ and so we may write this as

$$J^\mu = c\overline{\psi}\gamma^\mu\psi, \tag{6.13}$$

which shows that $\overline{\psi}\gamma^\mu\psi$ is a 4-vector.

The density and current satisfy the conservation (continuity) equation

$$\frac{\partial\rho}{\partial t} = -\boldsymbol{\nabla}\cdot\mathbf{J}, \tag{6.14}$$

which becomes simply

$$\partial_\mu J^\mu = c\partial_\mu\left(\overline{\psi}\gamma^\mu\psi\right) = 0. \tag{6.15}$$

Let us verify this directly from the Dirac equation. (For simplicity, from now on we use natural units.) We have

$$\partial_\mu\left(\overline{\psi}\gamma^\mu\psi\right) = \left(\partial_\mu\overline{\psi}\right)\gamma^\mu\psi + \overline{\psi}\gamma^\mu\partial_\mu\psi. \tag{6.16}$$

Now the Dirac equation gives $\gamma^\mu\partial_\mu\psi = -im\psi$, so

$$\overline{\psi}\gamma^\mu\partial_\mu\psi = -im\overline{\psi}\psi. \tag{6.17}$$

Taking the adjoint of the Dirac equation gives

$$(\partial_\mu\psi^\dagger)(\gamma^\mu)^\dagger = +im\psi^\dagger. \tag{6.18}$$

From the definition of the γ^μ matrices in terms of the hermitian α_j and β matrices, one may readily verify that

$$(\gamma^\mu)^\dagger = \gamma^0\gamma^\mu\gamma^0, \tag{6.19}$$

and hence

$$\left(\partial_\mu\psi^\dagger\right)(\gamma^\mu)^\dagger = \left(\partial_\mu\overline{\psi}\right)\gamma^\mu\gamma^0 = +im\psi^\dagger. \tag{6.20}$$

Thus, multiplying both sides on the right by γ^0 and using $(\gamma^0)^2 = 1$,

$$\left(\partial_\mu\overline{\psi}\right)\gamma^\mu = +im\overline{\psi}, \tag{6.21}$$

which, together with Eq. (6.17), shows that

$$\partial_\mu J^\mu = \partial_\mu\left(\overline{\psi}\gamma^\mu\psi\right) = +im\overline{\psi}\psi - im\overline{\psi}\psi = 0. \tag{6.22}$$

6.1 Dirac Lagrangian and Hamiltonian

Now we want to formulate the Lagrangian density $\mathcal{L}$ which has the Dirac equation as its equation of motion. A suitable choice is

$$\mathcal{L} = i\overline{\psi}\gamma^\mu\partial_\mu\psi - m\overline{\psi}\psi. \tag{6.23}$$

This is a choice in the sense that, as usual, we are free to add a total derivative. For example we could add $-\frac{i}{2}\partial_\mu\left(\overline{\psi}\gamma^\mu\psi\right)$ and write $\mathcal{L}$ in a more symmetrically pleasing (yet equivalent) form:

$$\mathcal{L} = \frac{i}{2}\left[\overline{\psi}\gamma^\mu\partial_\mu\psi - \left(\partial_\mu\overline{\psi}\right)\gamma^\mu\psi\right] = m\overline{\psi}\psi. \tag{6.24}$$

Just as we must treat φ and φ^* as independent fields in the Klein-Gordon case, we have to treat ψ and $\overline{\psi}$ as independent here. Using the Lagrangian density (6.23), the equation of motion for $\overline{\psi}$ gives the Dirac equation for ψ directly:

$$\partial_\mu\frac{\partial\mathcal{L}}{\partial(\partial_\mu\overline{\psi})} = 0 = \frac{\partial\mathcal{L}}{\partial\overline{\psi}} = i\gamma^\mu\partial_\mu\psi - m\psi, \tag{6.25}$$

while that for ψ gives the corresponding equation (6.21) for $\overline{\psi}$:

$$\partial_\mu\frac{\partial\mathcal{L}}{\partial\partial_\mu\psi} = i\left(\partial_\mu\overline{\psi}\gamma^\mu\right) = \frac{\partial\mathcal{L}}{\partial\psi} = -m\overline{\psi}. \tag{6.26}$$

You should check that the Lagrangian density (6.24) gives the same results. Note that when ψ and $\overline{\psi}$ satisfy their equations of motion, $\mathcal{L} = 0$. In other words, the minimum value of the action is zero.

The Hamiltonian density is

$$\mathcal{H} = \pi\frac{\partial\psi}{\partial t} + \frac{\partial\overline{\psi}}{\partial t}\overline{\pi} - \mathcal{L}, \tag{6.27}$$

where π and $\overline{\pi}$ are the canonical momentum densities conjugate to ψ and $\overline{\psi}$, respectively. Note that we have been careful with the order of factors: if ψ is represented by a column vector then pi is a row vector, and conversely for $\overline{\psi}$ and $\overline{\pi}$. Sticking with the simpler form (6.23) of the Dirac Lagrangian density, we have

$$\pi = \frac{\partial\mathcal{L}}{\partial(\partial\psi/\partial t)} = -\overline{\psi}\gamma^0 = i\psi^\dagger, \quad \overline{\pi} = \frac{\partial\mathcal{L}}{\partial(\partial\overline{\psi}/\partial t)} = 0, \tag{6.28}$$

and so (in natural units)

$$\begin{aligned}\mathcal{H} &= i\psi^\dagger\frac{\partial\psi}{\partial t} - \mathcal{L} \\ &= \psi^\dagger(-i\boldsymbol{\alpha}\cdot\boldsymbol{\nabla} + \beta m)\psi,\end{aligned} \tag{6.29}$$

which is just what we would expect for the energy density, given the Dirac equation (6.1).

6.2 Global and Local Phase Symmetry

Like the Klein-Gordon Lagrangian, The Dirac Lagrangian is invariant with respect to a global (space-time independent) phase change in ψ:

$$\psi \to e^{-i\varepsilon}\psi, \quad \overline{\psi} \to e^{+i\varepsilon}\overline{\psi}, \tag{6.30}$$

or, for an infinitesimal change,

$$\psi \to \psi - i\varepsilon\psi, \quad \overline{\psi} \to \overline{\psi} + i\varepsilon\overline{\psi}. \tag{6.31}$$

The associated Noether current is the one we found already:

$$J^\mu = -i\frac{\partial\mathcal{L}}{\partial(\partial_\mu\psi)}\psi + i\overline{\psi}\frac{\partial\mathcal{L}}{\partial(\partial_\mu\overline{\psi})} = \overline{\psi}\gamma^\mu\psi + 0. \tag{6.32}$$

In the presence of an electromagnetic 4-potential A_μ we expect an interaction term $-eJ^\mu A_\mu$, so that the Lagrangian density becomes

$$\mathcal{L} = i\overline{\psi}\gamma^\mu(\partial_\mu + ieA_\mu)\psi \equiv i\overline{\psi}\gamma^\mu D_\mu\psi, \tag{6.33}$$

where $D_\mu = \partial_\mu + ieA_\mu$ is the covariant derivative introduced in Section 4.3. Then, just as in the case of the Klein-Gordon field, we see that $\mathcal{L}$ is invariant under a *local* (space-time dependent) phase change $\varepsilon(x)$ combined with a gauge change $A_\mu \to A_\mu + \partial_\mu\varepsilon/e$.

6.3 Stress-Energy Tensor, Angular Momentum and Spin

The stress-energy tensor for the Dirac field is obtained by following the steps in Section 4.5. Using the Lagrangian density (6.23),

$$T^{\mu\nu} = \frac{\partial\mathcal{L}}{\partial(\partial_\mu\psi)}\partial^\nu\psi - g^{\mu\nu}\mathcal{L} = i\overline{\psi}\gamma^\mu\partial^\nu\psi, \tag{6.34}$$

where we have used the fact that $\mathcal{L} = 0$ when ψ satisfies the equation of motion. One can readily verify from the Dirac equation and Eq. (6.21) that this is indeed conserved. However, we cannot define a *symmetric* stress-energy tensor for the Dirac field and so the construction of a conserved angular momentum is more complicated than for the scalar or electromagnetic field.

By analogy with Eq. (4.67) we may define

$$M^{\lambda\mu\nu} = x^\mu T^{\lambda\nu} - x^\nu T^{\lambda\mu} = i\overline{\psi}\gamma^\lambda(x^\mu\partial^\nu - x^\nu\partial^\mu)\psi. \tag{6.35}$$

We find that

$$\partial_\lambda M^{\lambda\mu\nu} = T^{\mu\nu} - T^{\nu\mu} = i\overline{\psi}(\gamma^\mu\partial^\nu - \gamma^\nu\partial^\mu)\psi \neq 0, \tag{6.36}$$

so this is not conserved. Correspondingly the *orbital angular momentum* defined by

$$\begin{aligned} L_i &= \frac{1}{2}\varepsilon_{ijk}\int \mathrm{d}^3\mathbf{r}\, M^{0jk} \\ &= \frac{i}{2}\varepsilon_{ijk}\int \mathrm{d}^3\mathbf{r}\,\overline{\psi}\gamma^0\Big(x^j\partial^k - x^k\partial^j\Big)\psi \\ &= -i\int \mathrm{d}^3\mathbf{r}\,\psi^\dagger(\mathbf{r}\times\boldsymbol{\nabla})_i\psi \end{aligned} \tag{6.37}$$

is not conserved.

Now consider the tensor

$$S^{\lambda\mu\nu} = \frac{i}{4}\overline{\psi}\gamma^{\lambda}(\gamma^{\mu}\gamma^{\nu} - \gamma^{\nu}\gamma^{\mu})\psi, \tag{6.38}$$

which has

$$\begin{aligned}\partial_\lambda S^{\lambda\mu\nu} &= \frac{i}{4}\Big(\partial_\lambda\overline{\psi}\Big)\gamma^{\lambda}(\gamma^{\mu}\gamma^{\nu} - \gamma^{\nu}\gamma^{\mu})\psi + \frac{i}{4}\overline{\psi}\gamma^{\lambda}(\gamma^{\mu}\gamma^{\nu} - \gamma^{\nu}\gamma^{\mu})\partial_\lambda\psi \\ &= -\frac{m}{4}\overline{\psi}(\gamma^{\mu}\gamma^{\nu} - \gamma^{\nu}\gamma^{\mu})\psi + \frac{i}{4}\overline{\psi}\gamma^{\lambda}(\gamma^{\mu}\gamma^{\nu} - \gamma^{\nu}\gamma^{\mu})\partial_\lambda\psi \\ &= -\frac{i}{4}\overline{\psi}(\gamma^{\mu}\gamma^{\nu} - \gamma^{\nu}\gamma^{\mu})\gamma^{\lambda}\partial_\lambda\psi + \frac{i}{4}\overline{\psi}\gamma^{\lambda}(\gamma^{\mu}\gamma^{\nu} - \gamma^{\nu}\gamma^{\mu})\partial_\lambda\psi,\end{aligned} \tag{6.39}$$

where we used the Dirac equation, $i\Big(\partial_\lambda\overline{\psi}\Big)\gamma^{\lambda} = -m\overline{\psi}$, and its adjoint, $m\psi = i\gamma^{\lambda}\partial_\lambda\psi$, to arrive at the final expression. From the algebra (6.7) of the γ-matrices we find

$$\begin{aligned}\gamma^{\lambda}\gamma^{\mu}\gamma^{\nu} &= -\gamma^{\mu}\gamma^{\lambda}\gamma^{\nu} + 2g^{\lambda\mu}\gamma^{\nu} \\ &= \gamma^{\mu}\gamma^{\nu}\gamma^{\lambda} + 2g^{\lambda\mu}\gamma^{\nu} - 2g^{\lambda\nu}\gamma^{\mu},\end{aligned} \tag{6.40}$$

and similarly,

$$\gamma^{\lambda}\gamma^{\nu}\gamma^{\mu} = \gamma^{\nu}\gamma^{\mu}\gamma^{\lambda} + 2g^{\lambda\nu}\gamma^{\mu} - 2g^{\lambda\mu}\gamma^{\nu}. \tag{6.41}$$

Therefore,

$$\partial_\lambda S^{\lambda\mu\nu} = i\overline{\psi}\Big(g^{\lambda\mu}\gamma^{\nu} - g^{\lambda\nu}\gamma^{\mu}\Big)\partial_\lambda\psi = i\overline{\psi}(\gamma^{\nu}\partial^{\mu} - \gamma^{\mu}\partial^{\nu})\psi, \tag{6.42}$$

and so

$$\partial_\lambda\Big(M^{\lambda\mu\nu} + S^{\lambda\mu\nu}\Big) = 0. \tag{6.43}$$

The extra piece of this conserved tensor corresponds to the *spin* contribution to the angular momentum, $\mathbf{S}$, where

$$S_i = \frac{1}{2}\varepsilon_{ijk}\int \mathrm{d}^3\mathbf{r}\, S^{0jk} = \frac{i}{8}\varepsilon_{ijk}\int \mathrm{d}^3\mathbf{r}\,\overline{\psi}\gamma^{0}\Big(\gamma^{j}\gamma^{k} - \gamma^{k}\gamma^{j}\Big)\psi, \tag{6.44}$$

or in terms of the α- and β-matrices

$$S_i = -\frac{i}{8}\varepsilon_{ijk}\int \mathrm{d}^3\mathbf{r}\,\psi^{\dagger}(\alpha_j\alpha_k - \alpha_k\alpha_j)\psi. \tag{6.45}$$

Therefore we define

$$[\alpha_j, \alpha_k] = \alpha_j\alpha_k - \alpha_k\alpha_j = 2i\varepsilon_{ijk}\Sigma_l \tag{6.46}$$

so that

$$\mathbf{S} = \int \mathrm{d}^3\mathbf{r}\,\psi^{\dagger}\left(\frac{1}{2}\boldsymbol{\Sigma}\right)\psi. \tag{6.47}$$

This is the relativistic version of the Pauli spin $\frac{1}{2}\langle\boldsymbol{\sigma}\rangle$, which has to be added to the orbital angular momentum (6.37) in order to get the conserved total angular momentum:

$$\mathbf{J} = \int \mathrm{d}^3\mathbf{r}\,\psi^{\dagger}\left[-i(\mathbf{r}\times\boldsymbol{\nabla}) + \frac{1}{2}\boldsymbol{\Sigma}\right]\psi. \tag{6.48}$$

(Notice the unfortunate overlapping notation: the 3-vector total angular momentum $\mathbf{J}$ is not to be confused with the spatial component of the 4-vector current J^{μ}.) The fact

that the spin and orbital contributions are not conserved separately shows that there is *spin-orbit coupling*.

In the conventional representation of the α-matrices

$$\alpha_j = \begin{pmatrix} 0 & \sigma_j \\ \sigma_j & 0 \end{pmatrix}, \tag{6.49}$$

where the 2×2 Pauli matrices σ_j satisfy

$$[\sigma_j, \sigma_k] = \sigma_j\sigma_k - \sigma_k\sigma_j = 2i\varepsilon_{ijk}\sigma_l. \tag{6.50}$$

Eq. (6.46) then give

$$\Sigma_l = \begin{pmatrix} \sigma_l & 0 \\ 0 & \sigma_l \end{pmatrix}, \tag{6.51}$$

which is indeed the natural 4×4 extension of the Pauli matrices.

6.4 Massless Relativistic Particles

The need for a 4-spinor description of the quantum mechanical wave equation is dictated by the requirement that it be relativistic invariant, combined with the presence of a dimensional parameter (the mass). An equation for relativistic massless particles can be written using 2-spinors ψ_2, in the form of a *Weyl equation*:

$$i\tilde{\gamma}^\mu \partial_\mu \psi_2 = 0, \tag{6.52}$$

where $\tilde{\gamma}^0 = I_2$ (the 2×2 identity matrix) and $\tilde{\gamma}^i = \sigma_i$. For a plane wave with definite momentum $\mathbf{p}$ and energy $\varepsilon = |\mathbf{p}|$, $\eta_p \sim e^{-ipx}$, the Weyl equation reduces to

$$(\hat{\mathbf{n}} \cdot \boldsymbol{\sigma})\eta_p = \eta_p, \tag{6.53}$$

where $\hat{\mathbf{n}} \equiv \mathbf{p}/|\mathbf{p}|$. Similarly for an antiparticle plane wave ξ_p,

$$(\hat{\mathbf{n}} \cdot \boldsymbol{\sigma})\xi_p = -\xi_p. \tag{6.54}$$

The operator $\hat{\mathbf{n}} \cdot \boldsymbol{\sigma}$ projects the spin of the (anti)particle onto the direction of motion. Such projection is called the *helicity* and the Weyl equation tells us that states with definite momentum are also helicity eigenstates. An example of this type of particles are *neutrinos*, which conventionally have negative helicity $-1/2$, whereas anti-neutrinos have positive helicity $+1/2$. As we have seen in Section 6.3, the spin and orbital angular momentum are not separately conserved. Only the total angular momentum $\mathbf{J} = \mathbf{L} + \mathbf{S}$ is conserved. However, since the latter is transverse to the direction of motion (recall $\mathbf{L} = \mathbf{r} \times \mathbf{p}$), then $\hat{\mathbf{n}} \cdot \mathbf{S} = \hat{\mathbf{n}} \cdot \mathbf{J}$ and the helicity is therefore conserved.

N.B.: whereas the 2-spinor description of massless neutrinos is sufficient, one must represent them as 4-spinors if they are to interact with relativistic massive particles. In such 4-spinor representation, the absence of mass is only accidental (as opposed to being a strict necessity in the 2-spinor representation), and in general interactions do produce a small but non-vanishing mass term.

6.5 Dirac Equation in an External Field

In Section 6.2 we have seen how to couple a Dirac field to an EM field. This is called *minimal coupling* and it corresponds to replacing p_μ with $p_\mu - eA_\mu$ in the Dirac equation:

$$\gamma^\nu(i\hbar\partial_\nu - eA_\nu)\psi - mc\psi = 0. \tag{6.55}$$

To make the physical significance of the different contributions more transparent, it is convenient to transform this first order equation into a second order one by applying on the left the operator $\gamma^\nu(i\hbar\partial_\nu - eA_\nu) + mc$ to obtain:

$$\left[\gamma^\mu\gamma^\nu(i\hbar\partial_\mu - eA_\mu)(i\hbar\partial_\nu - eA_\nu) - m^2c^2\right]\psi = 0. \tag{6.56}$$

The product of Dirac matrices can be written as

$$\gamma^\mu\gamma^\nu = \frac{1}{2}(\gamma^\mu\gamma^\nu + \gamma^\nu\gamma^\mu) + \frac{1}{2}(\gamma^\mu\gamma^\nu - \gamma^\nu\gamma^\mu) = g^{\mu\nu} + \sigma^{\mu\nu}. \tag{6.57}$$

The first term follows from the property in Eq. (6.7), where we omitted the 4×4 identity martix for simplicity. The second term is a 4×4 antisymmetric 'matrix', where each element is in turn a 4×4 matrix. Taking a poetic licence in notation, a few lines of algebra show that

$$\sigma^{\mu\nu} = \begin{pmatrix} 0 & \alpha_1 & \alpha_2 & \alpha_3 \\ & 0 & -i\Sigma_3 & i\Sigma_2 \\ & & 0 & -i\Sigma_1 \\ & & & 0 \end{pmatrix}, \tag{6.58}$$

where we used the standard representation for the γ matrices and one has to remember that $0, \alpha_i$, and Σ_i are all 4×4 matrices, as defined earlier.

Contracting an antisymmetric tensor with another tensor suppresses any symmetric component of the latter. Namely, $\sigma^{\mu\nu}M_{\mu\nu} = \sigma^{\mu\nu}(M_{\mu\nu} - M_{\nu\mu})/2$. Therefore,

$$\sigma^{\mu\nu}(i\hbar\partial_\mu - eA_\mu)(i\hbar\partial_\nu - eA_\nu) = \frac{1}{2}\sigma^{\mu\nu}[i\hbar\partial_\mu - eA_\mu, i\hbar\partial_\nu - eA_\nu] = -\frac{1}{2}ie\hbar F_{\mu\nu}\sigma^{\mu\nu}, \tag{6.59}$$

where $F_{\mu\nu}$ is the EM field tensor introduced in Section 3.8.

Combining these results, we arrive at the second order equation

$$\left[(i\hbar\partial_\mu - eA_\mu)^2 - \frac{ie\hbar}{2}F_{\mu\nu}\sigma^{\mu\nu} - m^2c^2\right]\psi = 0, \tag{6.60}$$

which can be expressed explicitly in terms of the EM fields $\mathbf{E}$ and $\mathbf{B}$ as

$$\left[\left(\frac{i\hbar}{c}\partial_t - \frac{e}{c}\phi\right)^2 - (i\hbar\boldsymbol{\nabla} + e\mathbf{A})^2 = m^2c^2 + e\hbar\boldsymbol{\Sigma}\cdot\mathbf{B} - ie\hbar\boldsymbol{\alpha}\cdot\mathbf{E}\right]\psi = 0. \tag{6.61}$$

As we shall see in the next section, the last two terms in the square brackets encompass not only the coupling between spin and magnetic field, but also the coupling between spin and orbital angular momentum (known as *spin-orbit* coupling).

By promoting the first order equation to second order, additional solutions are introduced that do not satisfy the original equation (the ones with the opposite sign of the mass term). Given a generic solution φ of the second order equation, it can always be reduced to a correct solution of the original first order Dirac equation $\psi = [\gamma(p - eA) + m]\varphi$.

N.B.: In this section we have chosen to apply the minimal coupling to the EM fields in the first order Dirac equation before deriving the second order equation. This gives the correct result and it should be noted that the two operations do not commute. Had we first obtained the second order equation and then coupled it to the EM fields by substituting p_μ with $p_\mu - eA_\mu$, we would have missed some of the terms.

6.6 The Non-Relativistic Low-Energy Limit

One of the (many) great successes of Dirac's equation was to allow us to derive from first principles Pauli's equation, a phenomenological description of half-integer quantum mechanical particles. Pauli's equation obtains straightforwardly as a lowest order non-relativistic expansion ($v/c \ll 1$) at low energies (namely, EM field strengths much weaker than the rest mass energy).

If we write $\psi = (\psi_+, \psi_-)^T$, where ψ_+ and ψ_- are 2-spinors, we see that in the non-rel limit $\psi_- \to (0,0)^T$. Indeed, expanding to lowest order, one obtains:

$$i\hbar\partial_t\psi_+ = \left[\frac{1}{2m}(\mathbf{p} - e\mathbf{A})^2 + e\phi - \frac{e\hbar}{2mc}\boldsymbol{\sigma}\cdot\mathbf{B}\right]\psi_+, \tag{6.62}$$

and

$$\psi_+ = \frac{1}{2mc}\boldsymbol{\sigma}\cdot(\mathbf{p} - e\mathbf{A})\psi_+. \tag{6.63}$$

A guided derivation of this result is proposed as one of the questions in the problem set at the end of the lecture notes. From the expansion, one recognises the *gyromagnetic ratio* e/mc, which for spin 1/2 particles takes twice the value of the magnetic moment due to orbital motion.

In this approximation, the conserved current $j^\mu = c\overline{\psi}\gamma^\mu\psi$ can be decomposed into a density $J^0 = c\psi^\dagger\psi \simeq c(\psi_+)^\dagger\psi_+$ (since terms of the order of $(\psi_-)^\dagger\psi_-$ should be neglected), and a 3-current

$$\mathbf{J} = c\psi^\dagger\boldsymbol{\alpha}\psi = c(\psi_-)^\dagger\boldsymbol{\sigma}\psi_+ + c(\psi_+)^\dagger\boldsymbol{\sigma}\psi_-. \tag{6.64}$$

Substituting Eq. (6.63) and its hermitian conjugate into the expression for the current,

$$\mathbf{J} = \frac{1}{2m}\Big\{\Big[(\mathbf{p} - e\mathbf{A})^\dagger\psi_+^\dagger\cdot\boldsymbol{\sigma}\Big]\boldsymbol{\sigma}\psi_+ + (\psi_+)^\dagger\boldsymbol{\sigma}[\boldsymbol{\sigma}\cdot(\mathbf{p} - e\mathbf{A})\psi_+]\Big\}, \tag{6.65}$$

after a few lines of algebra one obtains

$$\mathbf{J} = \frac{i\hbar}{2m}\Big(\psi_+\boldsymbol{\nabla}\psi_+^\dagger - \psi_+^\dagger\boldsymbol{\nabla}\psi_+\Big) - \frac{e}{m}\mathbf{A}\psi_+^\dagger\psi_+ + \frac{\hbar}{2m}\boldsymbol{\nabla}\times\Big(\psi_+^\dagger\boldsymbol{\sigma}\psi_+\Big). \tag{6.66}$$

[Hint: in order to derive this result, you may find it useful to take advantage of the relationship $(\boldsymbol{\sigma}\cdot\mathbf{a})(\boldsymbol{\sigma}\cdot\mathbf{b}) = \mathbf{a}\cdot\mathbf{b} + i\boldsymbol{\sigma}\cdot\mathbf{a}\times\mathbf{b}$; more specifically, the two corollary relations $\boldsymbol{\sigma}(\boldsymbol{\sigma}\cdot\mathbf{b}) = \mathbf{b} + i\mathbf{b}\times\boldsymbol{\sigma}$ and $(\boldsymbol{\sigma}\cdot\mathbf{a})\boldsymbol{\sigma} = \mathbf{a} + i\boldsymbol{\sigma}\times\mathbf{a}$ (recall the cyclical property of $\boldsymbol{\sigma}\cdot\mathbf{a}\times\mathbf{b}$).] This result is indeed in agreement with the expression, obtained in non-relativistic quantum mechanics, for the current of a particle moving in an EM field.

6.7 Further work: $\mathcal{O}(v^2/c^2)$ Corrections

Continuing the expansion in powers of v/c, one finds relativistic corrections that go beyond the expected non-relativistic quantum mechanical behaviour. The derivation is beyond the scope of these lecture notes and we present here only a brief review of some of the main results.

Assuming a stationary state for simplicity, one obtains the equivalent of a Schrödinger Hamiltonian, $\varepsilon\phi_{\rm Sch} = \hat{H}\phi_{\rm Sch}$, of the form

$$\hat{H} = \frac{\hat{\mathbf{p}}^2}{2m} + e\phi - \frac{\hat{\mathbf{p}}^4}{8m^3c^2} - \frac{e\hbar}{4m^2c^2}\boldsymbol{\sigma}\cdot\mathbf{E}\times\hat{\mathbf{p}} - \frac{e\hbar^2}{8m^2c^2}\boldsymbol{\nabla}\cdot\mathbf{E}. \tag{6.67}$$

The last three terms are the corrections of order $(v/c)^2$. The first one is a relativistic correction to the kinetic energy from the expansion of the difference: $\sqrt{\mathbf{p}^2c^2 - m^2c^4} - mc^2$. The second term is typically referred to as *spin-orbit* interaction energy, whereby a moving magnetic moment couples to an electric field. If the field is centrally symmetric, then $\mathbf{E} = -\hat{\mathbf{r}}\,\mathrm{d}\phi/\mathrm{d}r$ and the spin-orbit contribution is proportional to

$$\frac{1}{r}\frac{\mathrm{d}\phi}{\mathrm{d}r}\hat{\mathbf{l}}\cdot\hat{\mathbf{s}}, \tag{6.68}$$

where $\hat{\mathbf{l}}$ is the orbital angular momentum operator, and $\hat{\mathbf{s}}$ is the electron spin operator.

Considering the Coulomb potential for an electron moving around a nucleus, we can use Eq. (6.67) in perturbation theory (namely, averaging the Hamiltonian over the non-relativistic unperturbed state), to obtain the relativistic correction to the energy levels of the Hydrogen atom (the so-called *fine structure*).

Chapter 7

Phase Transitions and Critical Phenomena

Many of the ideas developed so far in this course (Hamiltonian formalism, classical field theory, spontaneous symmetry breaking, etc) have application in another very important area of physics: critical phenomena and phase transitions. In this section we introduce some of the basic ideas, then discuss the simple Ising model for ferromagnetism and finally describe the Ginzburg-Landau Theory of second order phase transitions. This has some similarities with the Higgs mechanism discussed in the previous section.

7.1 Introduction to Phase Transitions and Critical Phenomena

It is rare in physics to find examples of interacting many-particle systems which admit to a full and accessible microscopic description or exact mathematical treatment. More useful is a *hydrodynamic* (i.e. effective) description of the collective long-wavelength behaviour which subsumes information at the microscopic scale (for example, fluid dynamics).

The averaged (*coarse grained*) variables appropriate to these length and time scales are no longer the discrete set of particle degrees of freedom but rather slowly varying continuous *fields* describing the collective motion of a macroscopic set of particles.

The most striking consequence of interactions among particles is the appearance of new phases of matter whose collective behaviour bears little resemblance to that of a few particles. Transitions between these new phases typically correspond to singularities in the free energy or the partition function. Since the canonical partition function of a finite collection of particles is always analytic, phase transitions can only be associated with infinitely many particles, i.e. the thermodynamic limit. The study of phase transitions is thus related to finding the origin of various singularities in the free energy and characterising them.

The paradigmatic example that exhibits many of the properties we wish to study is the ferromagnet. Although ferromagnetism is a complex phenomenon, we can think in terms of a simple model in which electrons in an incomplete inner shell have their spins effectively aligned in one and the same direction. Since there is a magnetic moment associated with each spin, such alignment implies that all these magnetic moments add, thus producing a macroscopic magnet.

When a ferromagnet is heated above a certain critical temperature T_c, its magnetism disappears and the material becomes paramagnetic. The qualitative behaviour of the (spontaneous) magnetisation is shown in Fig. 7.1. That spontaneous magnetisation should exist at all is a remarkable phenomenon – the spin Hamiltonian is rotation-invariant and

there are no preferred directions in space. For $T < T_c$ there is a preferred direction, that of the magnetisation. This is another example of *spontaneous symmetry breaking*. The magnetisation is called the *order parameter* of the transition. The transition at T_c is continuous (but note the singular first derivative) – this is an example of a *second-order phase transition*.

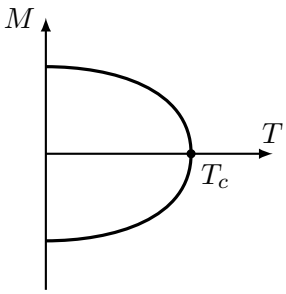

Fig. 7.1: Spontaneous magnetisation in a ferromagnet below the critical temperature T_c.

Experience tells us that a ferromagnet may abruptly change its macroscopic behaviour when the external conditions such as the temperature or magnetic field are varied. Consider what happens to the ferromagnet in the presence of an applied magnetic field B. The electron spins will align with the direction of the field, and so the magnetisation will depend on the magnitude and direction of the field. The dependence of the magnetisation M on the magnetic field B is shown in Fig. 7.2, for three different temperatures $T < T_c$, $T = T_c$ and $T > T_c$. For temperatures closer and closer to T_c, the size of the discontinuity decreases, until at $T = T_c$ the transition becomes continuous with $M = 0$ for $B = 0$. The same qualitative behaviour obtains for $T > T_c$, with the slope at $B = 0$ decreasing with increasing T.

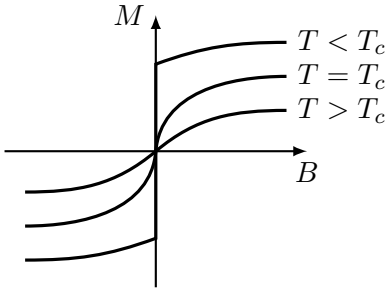

Fig. 7.2: Magnetisation M as a function of applied magnetic field B, for various values of temperature.

When the magnetic field changes at constant temperature $T < T_c$, the two states on either side of the critical point (spin up and spin down) coexist at the critical point. Such transitions involve discontinuous behaviour of thermodynamic properties and are termed *first-order* phase transitions.

In the vicinity of the critical point the *correlation length* – the characteristic length scale at which the overall properties of the system begin to differ markedly from those of the individual components — is large compared to the microscopic scales. Here we can use an effective theory involving only long-range collective fluctuations of the system. This suggests a Hamiltonian (or free energy) description constrained only by the fundamental symmetries of the system. This is called **Ginzburg-Landau theory**, and will

be discussed below. Although the detailed manner in which the material properties and microscopic couplings of the ferromagnet influence the parameters of the effective theory might be unknown, qualitative properties such as the *scaling behaviour* are completely defined.

7.2 Ising Model for Ferromagnetism

Consider a simple d-dimensional lattice of N classical 'spins' that can point up or down, $s_i = \pm 1$. Suppose there is an interaction J between nearest neighbour spins so that the parallel alignment is favoured ($J > 0$), with the Hamiltonian (energy)

$$H = -\frac{J}{2} \sum_{i,\delta} s_i s_{i+\delta} - \mu \sum_i s_i B. \tag{7.1}$$

Here the i sum runs over all sites in the lattice, and the δ sum runs over the nearest neighbours ($2d$ in a cubic lattice). The factor of $1/2$ in the first term is to avoid double counting the interaction, and the second term is the interaction of the moments μs_i with an external magnetic field B.

The canonical *partition function* is

$$Z = \sum_{\{s_i\}} e^{-\beta H(\{s_i\})} \qquad \left(\beta = \frac{1}{k_B T}\right), \tag{7.2}$$

summing the Boltzmann factor over all spin configurations $\{s_i\}$. Note that the enumeration of all configurations cannot be done for $d \geq 3$ and, although possible in $d = 2$, it is extremely hard there as well. Instead, we can use an approximate method of solution known as *mean field theory*.

For the simpler problem of non-interacting spins in a magnetic field described by the Hamiltonian

$$H_0 = -\mu \sum_i s_i B, \tag{7.3}$$

the partition function is simply the product of single spin partition functions

$$Z_0 = \left[e^{\beta b} + e^{-\beta b}\right]^N, \tag{7.4}$$

with $b = \mu B$, and the average spin on each site is

$$\langle s_i \rangle = \frac{e^{\beta b} - e^{-\beta b}}{e^{\beta b} + e^{-\beta b}} = \tanh(\beta b). \tag{7.5}$$

In the mean field approximation we suppose that the i^{th} spin sees an *effective field* b_{eff} which is the sum of the external field and the interaction from the neighbours calculated as if each neighbouring spin were fixed at its ensemble average value

$$b_{\text{eff}} = b + J \sum_\delta \langle s_{i+\delta} \rangle . \tag{7.6}$$

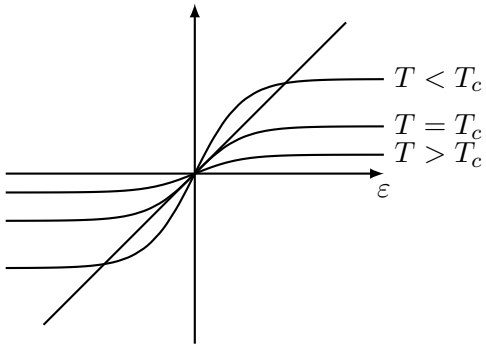

Fig. 7.3: Graphic solution of the self-consistent mean-field equation (7.8) for the Ising model, illustrating the qualitatively different behaviour for $T > T_c$, $T < T_c$, and $T = T_c$.

We now look for a *self-consistent* solution where each $\langle s_i \rangle$ takes on the same value s, which then has to satisfy, in analogy with (7.5),

$$s = \tanh\Big[\beta(b + 2dJs)\Big]. \tag{7.7}$$

[N.B.: You can alternatively think of mean field theory as a first order expansion in small flucutations of the spins with respect to their average value. Ignoring the fact that the spins take on discrete values, if most spins take a value close to their average s, then one can write the trivial identity $s_i = (s_i - s) + s$ and treat $s_i - s$ as a small parameter. Substituting this identiy into Eq. (7.1) and expanding to linear order in the small parameter, we obtain $H = -(Js/2)\Big(\sum_{i,\delta} s_i + \sum_{i,\delta} s_{i+\delta}\Big) = -2dJs \sum_i s_i$. Which reduces to the expected effective field contribution $b_{\text{eff}} = 2dJs$.]

Consider first $b = 0$. Define $\varepsilon = 2d\beta Js$ so that

$$\varepsilon = 2d\beta J \tanh \varepsilon, \tag{7.8}$$

with the temperature dependence entering through the β factor. This equation can be solved graphically (see Fig. 7.3), for example. For $T > T_c = 2dJ/k_B$, the only solution is $\varepsilon = 0$ (i.e., $s = 0$). For $T < T_c$ two new solutions develop (equal in magnitude but opposite in sign) with $|s|$ growing continuously below T_c. Near T_c (from below, i.e., $T < T_c$), $|\varepsilon| \ll 1$ and we can expand $\tanh \varepsilon$ in powers of ε, so that (7.8) becomes

$$\varepsilon = \frac{T_c}{T}\left(\varepsilon - \frac{1}{3}\varepsilon^3 + \cdots\right), \tag{7.9}$$

and the solution for s is

$$s = \pm\sqrt{3}\left(\frac{T_c - T}{T_c}\right)^{\frac{1}{2}} + \cdots, \tag{7.10}$$

to lowest order in $t = (T/T_c - 1)$, the *reduced temperature*. In general, the singular behaviour of the order parameter (in this case the magnetisation, proportional to s), is characterised by a *critical exponent* β (in this case $\beta = \frac{1}{2}$), i.e.

$$M(T, B \to 0^{\pm}) \propto |t|^{\beta} \quad \text{for} \quad T < T_c, \tag{7.11}$$

and $M = 0$ for $T > T_c$. (The critical exponent β should not be confused with $\beta = 1/k_B T$!)

We can also calculate the magnetic susceptibility, $\mathrm{d}M/\mathrm{d}B$, i.e. how the system responds to variations in the applied (small) magnetic field B. (This is an example of a *response function*, describing how the order parameter responds to an external perturbation.) Here we consider $\chi = \mathrm{d}s/\mathrm{d}b\,|_{b=0}$. Differentiating (7.7) gives

$$\frac{\mathrm{d}s}{\mathrm{d}b} = \mathrm{sech}^2\Big[\beta(b + 2Jds)\Big]\left(\beta + \frac{T_c}{T}\frac{\mathrm{d}s}{\mathrm{d}b}\right), \tag{7.12}$$

so that for T just above T_c

$$\chi = \frac{1}{k_B T_c}\left(\frac{T - T_c}{T_c}\right)^{-1}, \tag{7.13}$$

giving a *divergent* susceptibility as T approaches T_c from above, i.e. $\chi \propto |t|^{-\gamma}$ with the susceptibility exponent $\gamma = 1$ (in this simplified mean field theory approach).

For $T < T_c$ we must take the sponteous magnetisation $s_0 = \pm\sqrt{-3t}$ into account. Again by expanding the tanh function we can show that

$$\chi = \frac{1}{2k_B T_c}\left(\frac{T - T_c}{T_c}\right)^{-1}. \tag{7.14}$$

Evidently we have the same power γ but the numerical coefficients differ by a factor of 2.

Note that exactly at $T = T_c$ the relation between s and b is nonlinear:

$$s \simeq (\beta_c b + s) - \frac{1}{3}(\beta_c b + s)^3 + \cdots, \tag{7.15}$$

giving (the *critical isotherm*)

$$s(T = T_c, b) \simeq \left(\frac{3b}{k_B T_c}\right)^{\frac{1}{3}}, \tag{7.16}$$

where terms of order b^2, bs etc. have been ignored on the right-hand side of (7.15). The fact that $M \propto B^{1/\delta}$ along the critical point trajectory is quite general, although the result $\delta = 3$ is specific to the mean field theory approach.

Experimentally, it is found that the spontaneous magnetisation, the susceptibility and the critical isotherm (and the specific heat) all obey power laws near $T = T_c$ and one can measure the corresponding *critical exponents* (i.e. the exponents $\beta, \gamma, \delta, \cdots$, calculated above). Note that in the mean field approximation these exponents are independent of the number of spatial dimensions d. In general, because many states have quantitatively similar free energies as $T \to T_c$, fluctuations involving admixtures of states become important here and mean field theory will not in general be a good approximation. However it is often a useful first approach giving a qualitative prediction of the behaviour at phase transitions. It becomes exact, i.e. in agreement with the results of a full numerical calculation, when a large number of neighbouring sites participate in the interaction with each spin, since then the fluctuations in the effective field indeed become small compared with the mean. This happens in high enough d, or for long-range interactions.

In general, the thermodynamic critical properties of completely different physical systems can exhibit similar behaviour; for example, through the same dependence on temperature. In particular the critical point in the liquid-gas system is directly analogous to

the transition temperature in the Ising ferromagnet. The analogies are in fact quantitative – the transitions at the critical points are said to be in the same *universality class*. For example, the density discontinuity below the liquid-gas critical point grows as $(T_c - T)^\beta$, where β has the same value as in the growth of the magnetisation below T_c in the Ising ferromagnet and the compressibility in the gas diverges near T_c in the same way that the susceptibility does at the magnetic transition. The main difference between the two transitions is that the magnetic field B is an externally applied, symmetry-breaking field that can be set to zero. In the liquid-gas there is no symmetry difference between the two states below T_c (the dense liquid and rarefied gas), and the value of the pressure yielding the transition (corresponding to $B \to 0$ in the magnetic case) is not a priori obvious.

7.3 The Heisenberg Model

Consider the same lattice model as in the preceding section, but where the spins have unit length but are otherwise free to rotate in three dimensions, $\mathbf{s}_i = (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)$ in spherical polar coordinates, with the Hamiltonian ($J > 0$)

$$H = -\frac{J}{2}\sum_{i,\delta} \mathbf{s}_i \cdot \mathbf{s}_{i+\delta} - B\sum_i \hat{\mathbf{z}} \cdot \mathbf{s}_i. \tag{7.17}$$

Without loss of generality, we have chosen the direction of the field as the z axis of the reference frame for the spin direction. In zero field, H is symmetric under generic global rotations of the spins. If an ordered phase develops where $\langle \mathbf{s}_i \rangle \neq 0$, it breaks the symmetry by choosing a direction. As we shall see below, this happens spontaneusly for $B = 0$, but in presence of a finite field we expect the magnetisation to align with the field direction. Therefore, without loss of generality, we can assume that $\langle \mathbf{s}_i \rangle \equiv \mathbf{s} = s\hat{\mathbf{z}}$.

In the mean field approximation of small fluctuations about the average spin value, $|\mathbf{s}_i - \mathbf{s}| \ll 1$, we can expand the interaction energy of the system to linear order

$$\begin{aligned} H &= -\frac{J}{2}\sum_{i,\delta} [(\mathbf{s}_i - \mathbf{s}) + \mathbf{s}] \cdot [(\mathbf{s}_{i+\delta} - \mathbf{s}) + \mathbf{s}] - B\sum_i \hat{\mathbf{z}} \cdot \mathbf{s}_i \\ &\simeq -(2dJs + B)\sum_i \hat{\mathbf{z}} \cdot \mathbf{s}_i, \end{aligned} \tag{7.18}$$

and thus approximate the canonical *partition function* as

$$Z = \sum_{\{s_i\}} e^{-\beta H(\{s_i\})} \simeq \left[\int \mathrm{d}\cos\theta\, \mathrm{d}\phi\, e^{(2d\beta Js + \beta B)\cos\theta}\right]^N = (2\pi)^N \left[\int_{-1}^{1} \mathrm{d}x\, e^{(2d\beta Js + \beta B)x}\right]^N. \tag{7.19}$$

Similarly, we can obtain the average spin $\langle \mathbf{s}_i \rangle = \langle \mathbf{s}_i \cdot \hat{\mathbf{z}} \rangle\, \hat{\mathbf{z}}$

$$\begin{aligned} \langle \mathbf{s}_i \cdot \hat{\mathbf{z}} \rangle &= \frac{(2\pi)^N}{Z}\left[\int_{-1}^{1} \mathrm{d}x\, e^{(2d\beta Js + \beta B)x}\right]^{N-1}\left[\int_{-1}^{1} \mathrm{d}x\, e^{(2d\beta Js + \beta B)x}\right] \\ &= \frac{\int_{-1}^{1} \mathrm{d}x\, x e^{(2d\beta Js + \beta B)x}}{\int_{-1}^{1} \mathrm{d}x\, e^{(2d\beta Js + \beta B)x}} = -\frac{1}{\varepsilon + \beta B} + \coth(\varepsilon + \beta B), \end{aligned} \tag{7.20}$$

where we have introduced for convenience the shorthand notation $\varepsilon = 2d\beta Js$. The self-consistent mean field condition can finally be written as

$$s = -\frac{1}{2d\beta Js + \beta B} + \coth(2d\beta Js + \beta B), \tag{7.21}$$

or as

$$\varepsilon = 2d\beta J\left[-\frac{1}{\varepsilon + \beta B} + \coth(\varepsilon + \beta B)\right]. \tag{7.22}$$

Let us consider $B = 0$. Eq. (7.22) can then be studied graphically, as for the case of the Ising ferromagnet. The function on the r.h.s. behaves indeed similarly in the two cases and qualitatively one can refer to Fig. 7.3. Once again, we find a spontaneous symmetry breaking transition when the slope of the r.h.s. at $\varepsilon = 0$, $2d\beta J/3$, is equal to 1. Therefore, $T_c = 2dJ/3k_B$.

We can expand Eq. (7.22) for small s (small ε), as appropriate in proximity of the phase transition, to find ($T < T_c$)

$$\varepsilon = \frac{T_c}{T}\left(\varepsilon - \frac{1}{15}\varepsilon^3 + \cdots\right), \tag{7.23}$$

and the solution for s is

$$s = \pm\sqrt{\frac{5}{3}}\left(\frac{T_c - T}{T_c}\right)^{\frac{1}{2}} + \cdots \propto \pm|t|^{\beta}, \tag{7.24}$$

to lowest order in $t = (T/T_c - 1)$. Once again, we find the critical exponent $\beta = 1/2$.

We can obtain the magnetic susceptibility $\chi = \mathrm{d}s/\mathrm{d}b\,|_{b=0}$ by differentiating Eq. (7.21)

$$\chi = \beta(1 + 2dJ\chi)\left[\frac{1}{(2d\beta Js)^2} - \frac{1}{\sinh^2(2d\beta Js)}\right]. \tag{7.25}$$

For T just above T_c, s vanishes in the limit $B \to 0$ and the expansion in small s of the term in square brackets shows that it tends to the finite value 1/3,

$$\chi = \frac{1}{3k_B T_c}\left(\frac{T_c - T}{T_c}\right)^{-1}, \tag{7.26}$$

Notice the additional factor 1/3 in the coefficient.

At $T = T_c$, along the critical isotherm, for small B (hence small s) we can expand Eq. (7.21) to obtain the relation

$$s \simeq \frac{3s + \beta_c B}{3} - \frac{(3s + \beta_c B)^2}{45} + \cdots \quad \Longrightarrow \quad s(T = T_c, B) \simeq \left(\frac{5B}{9k_B T_c}\right)^{\frac{1}{3}}, \tag{7.27}$$

giving once again the mean field critical exponent $\delta = 3$.

7.4 Ginzburg-Landau Theory of Second Order Phase Transitions

Second order phase transitions occur when a new state of reduced symmetry develops continuously from the disordered (high temperature) phase, across a singularity in the free energy of the system. The ordered phase has a lower symmetry than the Hamiltonian – the phenomenon of *spontaneously broken symmetry*. In the broken symmetry phase, there is a number (sometimes infinite) of equivalent (e.g. equal free energy) symmetry-related states. These are macroscopically different, and so thermal fluctuations will not connect one to another in the thermodynamic limit. To describe the ordered state we need to introduce a macroscopic *order parameter* that describes the character and strength of the broken symmetry.

For example, for the Ising ferromagnet the Hamiltonian is invariant under all $s_i \to -s_i$, whereas the low-temperature phase has a spontaneous magnetisation, and so it is not invariant. A convenient order parameter in this case is the total average spin $S = \sum_i \langle s_i \rangle$ or the (total) magnetisation $M = \mu S$. This reflects the nature of the ordering: under the transformation $s_i \to -s_i$ we have $S \to -S$, and M goes to zero continuously at the critical temperature T_c.

Note that, for the more complicated case of the Heisenberg ferromagnet, the Hamiltonian is invariant under any rotation of all the spin vectors together and the ordering is characterised by a *vector* order parameter. A convenient choice is again the total spin $\mathbf{S} = \sum_i \langle \mathbf{S}_i \rangle$ or magnetisation $\mathbf{M} = \mu \mathbf{S}$.

Now consider the magnetic properties of a metal, say, close to the critical (Curie) temperature. The degrees of freedom that describe the transition are long-range collective excitations of spins. It is therefore appropriate to coarse-grain the magnet to a scale much larger than the lattice (i.e. atomic) spacing, and consider the vector magnetisation $\mathbf{m}(\mathbf{x})$ – the average of the elemental spins in the neighbourhood of the point $\mathbf{x}$. In other words, we are interested in the *vector field* $\mathbf{m}$, rather than the individual spins.

In other types of phase transitions, the role of $\mathbf{m}(\mathbf{x})$ is played by the appropriate order parameter. The dimension n of $\mathbf{m}(\mathbf{x})$ need not be the same as the spatial dimension d of $\mathbf{x}$. For example, for liquid-gas or Ising transitions $n = 1$, for superfluidity $n = 2$, and for classical (isotropic or Heisenberg) magnets $n = 3$. Likewise we can consider phase transitions in wires ($d = 1$) and on surfaces ($d = 2$).

Ginzburg-Landau theory provides a phenomenological description of critical phenomena applicable in the general case. The key quantity is the coarse-grained, effective free energy Hamiltonian for the system, regarded as a function of $\mathbf{m}(\mathbf{x})$ and its derivatives, rather then the microscopic Hamiltonian of, for example, the Ising model discussed above. It is constructed on the basis of *symmetries*, rather than precise knowledge of the microscopic properties of the system.

7.4.1 Free Energy Expansion

The free energy must be invariant under all relevant symmetry operations of the Hamiltonian, whose dependence on the order parameter is therefore constrained. In particular, the Hamiltonian should have translational and rotational symmetry in $\mathbf{x}$ space, and rotational symmetry in $\mathbf{m}$ space, i.e. under rotations $\mathbf{m} \to_n \mathbf{m}$. This leads to the general form

$$A = \beta H = \int \mathrm{d}^d\mathbf{x}\, f(\mathbf{m}(\mathbf{x}), \boldsymbol{\nabla}\mathbf{m}, T), \tag{7.28}$$

where the free energy density f is a function of the local order parameter $\mathbf{m}$, its spatial derivatives, temperature T and other external parameters such as the magnetic field $\mathbf{B}$ in the case of ferromagnets. Note that $(\boldsymbol{\nabla}\mathbf{m})_{ij} = \partial m_j/\partial x_i$ with $i = 1, \cdots, d$ and $j = 1, \cdots, n$, but of course f must be a scalar quantity in terms of both types of indices.

Although there is a strong (and often useful) similarity between (7.28) and the Hamiltonian formulation of classical mechanics encountered earlier, one ought to have a clear understanding of the differences. What we refer to as 'Hamiltonian' in this section is an effective description of the free energy of the system *in thermodynamic equilibrium*. As such, there is no notion of dynamics or time dependence here (note that indeed only *spatial* derivatives of the field $\mathbf{m}(\mathbf{x})$ appear in this Hamiltonian). Whereas minimising the action in classical mechanics allowed one to obtain the equations of motion of the system (i.e., its preferred 'space-time trajectory'), minimising the free energy (7.28) gives the most thermodynamically favourable state of the system. It would of course make no sense at all to try and use (7.28) to obtain equations of motion!

Near the transition temperature ($|\mathbf{m}|$ small) we can expand f in powers of $\mathbf{m}$ (and its derivatives):

$$f = f_0(T) + \alpha(T)\mathbf{m}^2 + \frac{1}{2}\beta(T)\mathbf{m}^4 + \cdots + \gamma(T)(\boldsymbol{\nabla}\mathbf{m})^2 + \delta(T)(\boldsymbol{\nabla}\mathbf{m})^4 + \cdots, \tag{7.29}$$

where $\alpha, \beta, \cdots$, are non-universal phenomenological parameters determined by the microscopic properties of the system. The probability of a particular configuration is $\propto \exp(-\beta H)$, but in general these parameters are *not* proportional to $(k_B T)^{-1}$.

For the specific example of the Ising ferromagnet in the absence of an applied magnetic field, the order parameter is the scalar field $m(\mathbf{x})$, i.e. $n = 1$, the magnetisation per unit volume or the magnetisation per spin averaged over some reasonably macroscopic volume. In this case

$$f(m, T) = f_0(T) + \alpha(T)m^2 + \frac{1}{2}\beta(T)m^4 + \gamma(T)\boldsymbol{\nabla}m \cdot \boldsymbol{\nabla}m + \cdots, \tag{7.30}$$

where the term involving spatial derivatives of m corresponds to the free energy cost of a nonuniform m. In the discrete (lattice) space case, it corresponds to nearest-neighbour interactions of the form

$$\sum_{i,\mu} \frac{1}{a^2}[m(\mathbf{x}_i + \boldsymbol{\mu}) - m(\mathbf{x}_i)]^2 \tag{7.31}$$

where a is the lattice spacing, i labels the lattice points, and the vector $\boldsymbol{\mu}$ links nearest neighbours. The choice of $\gamma > 0$ ensures that the spatially uniform state gives the lowest value of the free energy A.

Sixth and higher order terms in m could be retained in (7.30), but are not usually necessary for the important behaviour near the transition temperature T_c. Note that we do keep the fourth order term, because at T_c the coefficient of the second-order term $\alpha(T)$ becomes zero, as discussed below. Only quadratic derivative terms are usually needed, since generally $\gamma(T_c)$ is positive and therefore the order parameter can be assumed to be smoothly varying in $\mathbf{x}$.

7.4.2 Minimum Free Energy

We expect the state that minimises the free energy to be the physically realized state. This is true so long as the fluctuations around this most probable value are small compared to this value. This is not always the case, and Ginzburg-Landau theory then corresponds to a mean field theory that ignores these fluctuations. For the Ising ferromagnet with zero external magnetic field B, the minimum of A, after substituting (7.30) into (7.28), is given by a uniform $m(\mathbf{x}) = \bar{m}$ satisfying

$$\alpha\bar{m} + \beta\bar{m}^3 = 0. \tag{7.32}$$

The solutions corresponding to a minimum are

$$\bar{m} = \pm\sqrt{-\alpha/\beta} \quad \text{for} \quad \alpha < 0, \quad \text{and} \quad \bar{m} = 0 \quad \text{for} \quad \alpha > 0. \tag{7.33}$$

Comparing (7.33) with (7.10) suggests that we can identify $\alpha = 0$ as where the temperature passes through T_c, and expand about $T = T_c$,

$$\begin{aligned} \alpha(T) &\simeq a(T - T_c) + \cdots \\ \beta(T) &\simeq b + \cdots \\ \gamma(T) &\simeq c + \cdots, \end{aligned} \tag{7.34}$$

so that

$$f(m,t) \simeq f_0(T) + a(T - T_c)m^2 + \frac{1}{2}bm^4 + c\boldsymbol{\nabla}m \cdot \boldsymbol{\nabla}m, \tag{7.35}$$

and

$$\bar{m} \simeq \pm\left(\frac{a}{b}\right)^{\frac{1}{2}}\sqrt{(T_c - T)} \quad \text{for} \quad T < T_c. \tag{7.36}$$

Evaluating f at $\bar{m}$ gives

$$\bar{f} = f_0 - \frac{a^2(T - T_c)^2}{2b}, \tag{7.37}$$

showing the lowering of the free energy by the ordering (one can easily verify that $\bar{f} = f_0$ for $T = T_c$).

We can gain useful insight into the transition by plotting f in (7.35) for a uniform m at various temperatures, as in Fig. 7.4. For $T > T_c$ the free energy has a single minimum at $m = 0$. Below T_c two new minima at $\bar{m} = \pm\sqrt{a(T_c - T)/b}$ develop. At $T = T_c$ the curve is very flat at the minimum (varying as m^4) and fluctuations are expected to be particularly important here.

Next, we consider adding the coupling to a magnetic field B.

$$f(m,T,B) \simeq f_0(T) + a(T - T_c)m^2 + \frac{1}{2}bm^4 + c\boldsymbol{\nabla}\mathbf{m} \cdot \boldsymbol{\nabla}\mathbf{m} - mB. \tag{7.38}$$

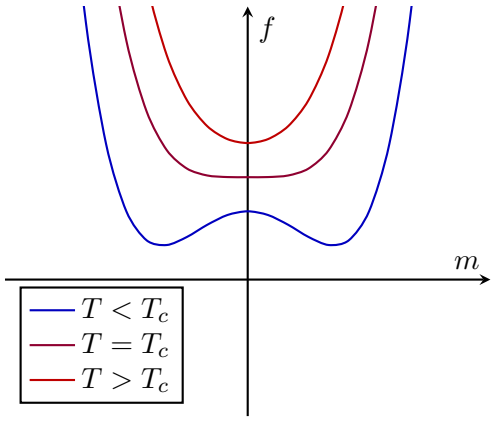

Fig. 7.4: Free energy density f as a function of (uniform) m, for various values of temperature T.

The magnetic field couples directly to the order parameter and is a *symmetry breaking* field: with the addition of the mB term, the full Hamiltonian is no longer invariant under spin inversion. The free energy is now minimised by a non-zero m in the direction of B ($m > 0$ if $B > 0$, and vice versa). Minimising f again with respect to m, we find that for $T > T_c$ the susceptibility diverges:

$$\chi = \left.\frac{\mathrm{d}\bar{m}}{\mathrm{d}B}\right|_{B=0} = \frac{1}{2a}(T - T_c)^{-1}. \tag{7.39}$$

(Hint: to derive this expression, first obtain the equivalent of (7.32) from (7.38); then take the derivative with respect to B and find χ as a function of $\bar{m}^2$. Finally, substitute for $\bar{m}^2$ evaluated at $B = 0$, which we already derived earlier. How does the behaviour of the susceptibility χ change for $T < T_c$?)

At $T = T_c$ for small B,

$$\bar{m} = \left(\frac{1}{2b}\right)^{1/3} B^{1/3}. \tag{7.40}$$

Note that the exponents (power laws) are the same as we found in the direct mean field theory calculation for the Ising model.

Finally, for a complex scalar order parameter $m \neq m^*$, we can perform a Taylor expansion in $\mathrm{Re}\{m\}$ and $\mathrm{Re}\{m\}$, and demand the invariance of each term under a change of the phase. This leads to the form

$$f = f_0 + a(T - T_c)|m|^2 + \frac{1}{2}b|m|^4 + c\boldsymbol{\nabla}m \cdot \boldsymbol{\nabla}m^*. \tag{7.41}$$

Note that a term in $|m|^3$ is not allowed, even though it is invariant under a phase transformation, since it does not correspond to a term in the Taylor expansion of the real and imaginary parts of m. The similarity with the Higgs potential Hamiltonian density (5.2, 5.3) is striking and illustrates how the phenomenon of spontaneous symmetry breaking can be manifest in completely different physical systems.

7.5 First Order Phase Transitions

The Landau-Ginzburg free energy formalism describes not only continuous phase transitions, but also first order transitions. This is the case for instance of a liquid-solid transition where the order parameter is the density ρ of the liquid. In this case, there is no symmetry in changing the sign of the density and cubic terms are allowed in the free energy expansion. Assuming for simplicity a uniform density,

$$f = f_0 + a(T - T_c)\rho^2 + c\rho^3 + \frac{b}{2}\rho^4, \tag{7.42}$$

whose behaviour is represented schematically in Fig. 7.5(a). At high temperatures there is a single minimum at $\rho = 0$ corresponding to the liquid phase. As the temperature is lowered, a second minumum develops at $\rho \neq 0$. Its free energy is initially higher than the liquid, and the new phase is therefore considered metastable. For $T < T_m$ the new free energy minimum becomes lower than the minimum at $\rho = 0$. Tm is the melting, or coexistence, temperature where the liquid and solid phases have the same free energy. At T_m the value of the order parameter ρ jumps discontinuously, in contrast to the behaviour at a continuous phase transition. Notice that there is a temperature window $T_c < T < T_m$ where the minimum at $\rho = 0$ survives, albeit being only a local minimum (metastable). It disappears only for $T < T_c$, when the liquid state no longer exists.

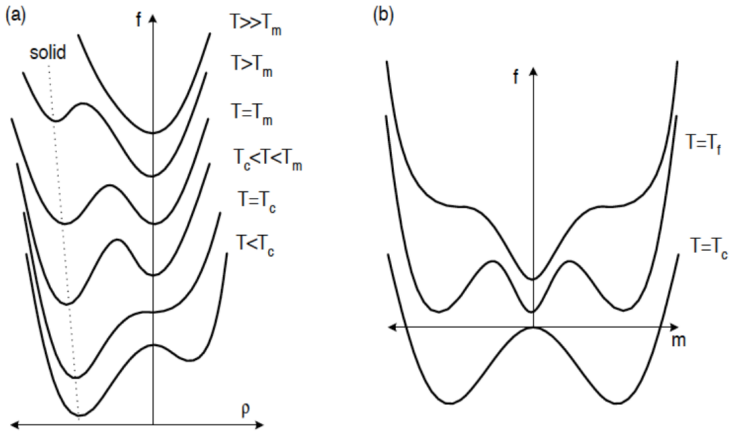

Fig. 7.5: Behaviour of the Free energy when (a) a cubic term is included; and (b) in the case where the coefficient of the quartic term is negative.

Alternatively, first order transitions can arise in the absence of cubic terms, when the coefficient of the quartic term happens to be *negative*. In this case, we need a *sixth* (or higher) order term with positive coefficient to ensure that the free energy is bounded from below. Again, assuming the order parameter m to be uniform for simplicity,

$$f = f_0 + a(T - T_c)m^2 - \frac{b}{2}m^4 + \frac{c}{3}m^6, \tag{7.43}$$

which is illustrated in Fig. 7.5(b). In this case, two symmetric secondary minima develop as the temperature is lowered. They are initially metastable, and they become the lowest minima at T_f, the first order transition temperature. Here the order parameter jumps discontinuously from $m = 0$ to a finite value of m, at is *spontaneously breaks the symmetry* between the two new minima. Once again, the $m = 0$ phase survives as a secondary (metastable) minimum below T_f and disappears only at some lower temperauture T_c.

N.B.: The Landau-Ginzburg description is not necessarily accurate at first order transitions. Since there is a jump in the order parameter, there is no guarantee that the truncated expansion be a reasonable approximation. Although it is useful to illustrate the qualitative behaviour, it can give misleading conclusions.

Chapter 8

Propagators and causality

In quantum mechanics at the Schrödinger level, propagators offer a direct way to include interactions and other complexities using perturbation theory. However, the mathematical concept of cause and effect, with the *propagator* playing the role of a messenger function connecting the two, is applicable to a far broader range of problems. Let us consider, as an introductory example, the classical Lagrangian system of a simple harmonic oscillator.

8.1 Simple Harmonic Oscillator

Consider a discrete particle characterised by its coordinate $x(t)$, in a harmonic potential, possibly subjected to an external driving force $f(t)$. The Lagrangian is

$$L = T - V = \frac{m}{2}\left(\frac{\mathrm{d}x}{\mathrm{d}t}\right)^2 - \frac{1}{2}\kappa x^2 + xf(t). \tag{8.1}$$

The Euler-Lagrange condition for the minimal action leads to the familiar differential equationn

$$\frac{\mathrm{d}^2x}{\mathrm{d}t^2} + \omega_0^2 x + \phi(t) \quad \text{with} \quad \omega_0^2 = \frac{\kappa}{m}, \quad \phi = \frac{1}{m}\phi(t) \tag{8.2}$$

We can of course solve the problem directly when the external force is a simple cosine function, $f(t) = f_0\cos(\Omega t)$. Let us, however, explore the role of a causal propagator in more general terms. Define the propagator (or Green's function in this context) as the solution of

$$\left[\frac{\mathrm{d}^2}{\mathrm{d}t^2} + \omega_0^2\right] G(t-t') = \delta(t-t'), \tag{8.3}$$

or in Fourier-transformed form

$$\left[-\omega^2 + \omega_0^2\right] G(\omega) = 1 \quad \text{for} \quad G(t-t') = \int G(\omega) e^{-i\omega(t-t')} \frac{\mathrm{d}\omega}{2\pi}. \tag{8.4}$$

The physical meaning of this function is the response to an impulse force, $\delta(t-t')$, which occurred at the moment of time t'. Causality demands that there should be no response before the moment $t = t'$, so

$$G(t-t') = \int \frac{e^{-i\omega(t-t')}}{\omega_0^2 - \omega^2} \frac{\mathrm{d}\omega}{2\pi} \qquad \text{when } t > t', \tag{8.5}$$

$$G(t-t') = 0, \qquad \text{when } t < t'. \tag{8.6}$$

Then the solution of (8.2) can be formally written as

$$x(t) = \int G(t-t')\phi(t')\,\mathrm{d}t', \quad \text{a convolution in real time} \tag{8.7}$$

$$\text{or} \quad x(t) = \int x(\omega) e^{-i\omega t} \frac{\mathrm{d}\omega}{2\pi}, \quad \text{with } x(\omega) = G(\omega)\phi(\omega) \text{ in Fourier representation} \tag{8.8}$$

which may require some contour integration in the complex plane of ω, since $G(\omega)$ has two simple poles at $\omega = \pm\omega_0$. Let us illustrate this procedure in an explicit example.

8.1.1 Damped Oscillator

The explicit calculation of the propagator is, perhaps paradoxically, easier in the case when the oscillator is damped. We take the equation (8.2) and add the frictional force to it,

$$\frac{\mathrm{d}^2x}{\mathrm{d}t^2} + \gamma\frac{\mathrm{d}x}{\mathrm{d}t} + \omega_0^2 x = \phi(t). \tag{8.9}$$

The Green's function is the solution of the corresponding equation with a δ-function source

$$\left[\frac{\mathrm{d}^2}{\mathrm{d}t^2} + \gamma\frac{\mathrm{d}}{\mathrm{d}t} + \omega_0^2\right] G(t-t') = \delta(t-t') \tag{8.10}$$

$$\left[-\omega^2 - i\gamma\omega + \omega_0^2\right] G(\omega) = 1, \quad \text{for} \quad G(t-t') = \int G(\omega) e^{-i\omega(t-t')} \frac{\mathrm{d}\omega}{2\pi}. \tag{8.11}$$

The causal propagator should satisfy the requirement that there be no motion until the force is applied at $t = t'$

$$G(t-t') = \int_{-\infty}^{\infty} \frac{e^{-i\omega(t-t')}}{\omega_0^2 - i\gamma\omega - \omega^2} \frac{\mathrm{d}\omega}{2\pi} \qquad \text{for} \quad t > t' \tag{8.12}$$

$$G(t-t') = 0 \qquad \text{for} \quad t < t' \tag{8.13}$$

(obviously, we require that the damping is positive, $\gamma > 0$). This is a classic case for contour integration in the complex plane of frequency ω. The integrand in (8.12) has two simple poles at the roots of the denominator,

$$\omega_{1,2} = -\frac{i\gamma}{2} \pm \sqrt{\omega_0^2 - \frac{\gamma^2}{4}}. \tag{8.14}$$

When $\gamma_0^2 > \gamma^2 > 4$ these two poles lie in the lower half of the ω complex plane, shifted down from the real axis by $\gamma/2$ (compare with Eq. (8.5) where they lie on the real axis). The trick is to make a closed integration contour by adding the semi-circular arc $\omega = Re^{i\varphi}$ for $R \to \infty$ and the phase $\varphi = \{0, \pi\}$ when you close the contour in the upper half-plane ($\mathcal{C}_+$), or $\varphi = -\{0, \pi\}$ when the contour is closed in the lower half-plane ($\mathcal{C}_-$), in both cases connecting the points $\omega = +\infty$ and $-\infty$ on the real axis, as required in (8.12). The two contours are illustrated in Fig. 8.1.

When $t - t' > 0$, the argument of the Fourier exponential in (8.12) is $-i|t-t'|Re^{i\varphi}$. On the upper half-plane arc $\mathcal{C}_+$, its real part is positive and the contribution to the integral diverges as $R \to \infty$, so we are not allowed to add $\mathcal{C}_+$ to the contour. In contrast, on the lower half-plane arc $\mathcal{C}_-$, its real part is negative and the contribution to the integral vanishes as $R \to \infty$, so we are free to close the contour in the lower half-plane by adding $\mathcal{C}_-$. This does not alter the desired result for $G(t-t')$ and, by Cauchy's theorem, it is equal to $(2\pi i) \times$ [sum of *residues*] of the poles enclosed, which conveniently do lie inside this contour. Note that the contour $\mathcal{C}_-$ is clockwise, in the "wrong" direction, hence there

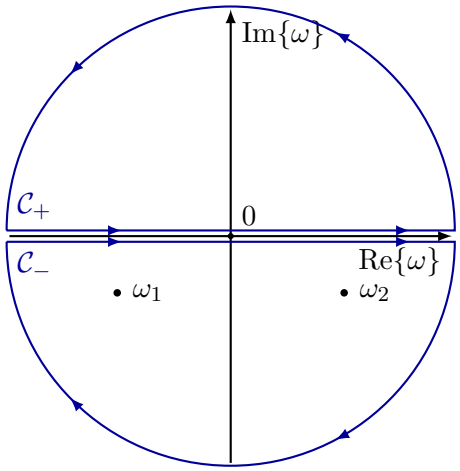

Fig. 8.1: Closing the contour in the upper and the lower half-planes makes a difference on whether the poles are enclosed.

is an extra minus sign:

$$G(t>t') = \oint_{\mathcal{C}_-} \frac{e^{-i\omega(t-t')}}{\omega_0^2 - i\gamma\omega - \omega^2}\frac{\mathrm{d}\omega}{2\pi} = -2\pi i\Big[\mathrm{res}\{\omega=\omega_1\} + \mathrm{res}\{\omega=\omega_2\}\Big] \tag{8.15}$$

$$= \frac{i}{\omega_1-\omega_2}\Big[e^{-i\omega_1(t-t')} - e^{-i\omega_2(t-t')}\Big]$$

$$= \frac{1}{\sqrt{\omega_0^2-\gamma^2/4}} e^{-(\gamma/2)|t-t'|}\sin\Big(\sqrt{\omega_0^2-\gamma^2/4}|t-t'|\Big) \quad \text{for} \quad t>t' \tag{8.16}$$

This shows how the oscillations gradually decay after being excited by an impulse at $t = t'$.

In the non-causal domain $t < t'$, by a similar argument the contour closure has to be done in the upper half-plane and the resulting contour $\mathcal{C}_+$ does not enclose the poles! Hence $G(t<t') = 0$.

This analysis of the damped oscillator allows us to recover the undamped oscillator as the limiting case $\gamma \to 0$, giving $G(t-t') \to \frac{1}{\omega_0}\sin[\omega_0(t-t')]$ in equations (8.3) and (8.7). Try examining the omitted cases, when the damping is too large ($\omega_0^2 < \gamma^2/4$) and when $\gamma < 0$ (negative damping). Trace where the poles move in the complex plane and how this affects the causal response.

8.2 Free Quantum Particle

The approach is exactly the same for more complicated systems as for instance the Schrödinger equation. One needs to separate the non-interacting part of the field $\psi(x,t)$ into the Schrödinger-like system:

$$i\hbar\frac{\partial\psi}{\partial t} + \frac{\hbar^2}{2m}\nabla^2\psi = F(x,t), \tag{8.17}$$

where $F(x,t)$ contains all the interaction terms (the source of the interesting physics but of the complications as well). The propagator G gives the solution for $\psi(t)$ due to

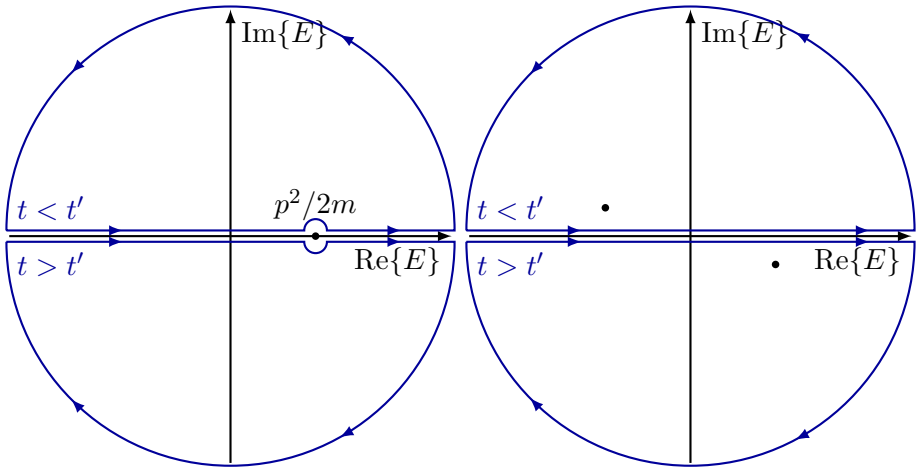

Fig. 8.2: The complex energy plane, illustrating the pole positions and integration contours.

interactions at earlier times. In quantum mechanics it is then defined as:

$$\psi(x,t) = \int_{t>t'} \mathrm{d}t' \int \mathrm{d}x'\, G(x,x';t,t')F(x',t'). \tag{8.18}$$

At this point it may be useful to remove a possible confusion in terminology. At least for equations of motion that are first order in $\partial/\partial t$, one can also define a propagator such that $\Psi(x,t) = \int \tilde{G}(x,x';t,t')\Psi(x',t')\,\mathrm{d}x'$, where $t > t'$ for the non-interacting equation. You can readily check that $\tilde{G} = i\hbar G$. In this sense, $\tilde{G}$ is the amplitude to propagate from x' to x in time $t - t'$.

Clearly, G in (8.18) is just a Green's function of the non-interacting equation,

$$\left(i\hbar\frac{\partial}{\partial t} + \frac{\hbar^2}{2m}\nabla^2\right)G(x,x';t,t') = \delta(x-x')\delta(t-t'). \tag{8.19}$$

By using momentum and energy representations, essentially the Fourier transforms through $\exp[-ipx/\hbar]$ and $\exp[-iEt/\hbar]$ (so that $q = p/\hbar$ and $\omega = E/\hbar$), we obtain:[1]

$$\left(i\hbar\frac{\partial}{\partial t} - \frac{p^2}{2m}\right)G(p;t,t') = \delta(t-t')$$

$$\left(E - \frac{p^2}{2m}\right)G(p;E) = 1 \tag{8.20}$$

$$G(p;t,t') = \int e^{-iE(t-t')/\hbar}\frac{1}{E - p^2/2m}\frac{\mathrm{d}E}{2\pi\hbar}, \tag{8.21}$$

with a single simple pole at $E = p^2/2m$ on the real axis. For $t > t'$ we must close the contour in the lower half-plane and for $t < t'$ in the upper half (to have e^{-z} at $z \to \infty$ in both cases).

[1] Warning on sign conventions: In QM the sign convention for oscillation with time is $\Psi(t) \propto \exp[-iEt/\hbar]$ whereas for ordinary oscillators and in the general Fourier analysis we use $u(t) \propto \exp[i\omega t]$. As a result, causal poles must lie above the contour for ω, as opposed to below for E. An easy way to sort out the sign convention is to remember that poles with positive damping should naturally be causal.

The principle of causality tells us that the contour must pass above the simple pole at $E = p^2/2m$:

$$G(p; t < t') \quad \text{must be zero} \tag{8.22}$$

$$G(p; t > t') = -2\pi i \left[\frac{1}{2\pi\hbar} e^{-i(t-t')(p^2/2m)/\hbar} \right] = -\frac{i}{\hbar} e^{-i\frac{p^2}{2m\hbar}(t-t')}. \tag{8.23}$$

In high energy physics it is common to use the "pole moving trick" to preserve the simplicity of $\int \mathrm{d}E$ over real values: move the singular point down into the lower half-plane, $E \to E + i\varepsilon$,

$$G(p; E) \to \frac{1}{E - p^2/2m + i\varepsilon}. \tag{8.24}$$

In relativistic quantum mechanics the "dispersion relationship" is $E^2 = p^2c^2 + m^2c^4$

$$G(p; E) \to \frac{1}{E^2 - p^2c^2 - m^2c^4 + i\varepsilon}, \tag{8.25}$$

and so the two poles at $E = \pm\sqrt{p^2c^2 + m^2c^4 - i\varepsilon}$ end up one in each half-plane! This seeming violation of causality (the contour closed in the "wrong" half-plane also produces a result) corresponds to real physics - the contributions of particles and antiparticles, which, as we saw in Section 4.7, give rise to the positive and negative frequency parts of the quantum field.

8.3 Linear Response and Kramers-Kronig Relations

A dynamical variable $u(t)$ with zero average, $\langle u \rangle = 0$, always has a conjugate force $f(t)$ defined so that the corresponding perturbation of the potential energy is $-uf$. This also applies to the physical fields entering the Lagrangian density. As a simple example, consider a particle on a spring with a potential $V(x) = \frac{1}{2}\kappa x^2$ (in equilibrium at $x = 0$). Applying an external force results in the perturbation of the potential so that $V' = V(x) - xf$. The new equilibrium is now at $\langle x \rangle_f = \frac{1}{\kappa} f$. We thus define a linear static response function $\alpha = \frac{1}{\kappa}$ in this example. Other familiar examples include those listed in Table 8.1.

u	f	
position	force	$-xf$
charge	voltage	$-q\varphi$
magnetic moment	magnetic induction	$-MB$
polarisation	electric field	$-PE$
volume	pressure	$-VP$

Table 8.1: Examples of conjugate forces $f(t)$ for dynamical variables $u(t)$ with zero average, $\langle u \rangle = 0$, such that the corresponding perturbation of the potential energy is $-uf$.

In fact, different thermodynamic potentials may have the inverse definition of a variable and its conjugate force, e.g. volume may be reduced by an externally applied pressure, or pressure may be changed by externally changing the volume. The concept of linear response function, connecting the small change in a quantity induced by its (small) conjugate force, remains valid in each case.

In most physical situations, one is faced with time-varying forces and responses. In this case we have

$$\langle u(t)\rangle_f = \int_{-\infty}^{\infty} \alpha(t-t')f(t')\,\mathrm{d}t' \tag{8.26}$$

$$\text{or} \quad \langle u(\omega)\rangle_f = \alpha(\omega)f(\omega) \quad \text{in the Fourier domain,} \tag{8.27}$$

with α the linear response function or *generalised susceptibility*. Causality demands that $\alpha(t-t')$ is finite only for $t > t'$ and is zero for $t < t'$, i.e. there is no response before the force is applied. This imposes a constraint on the real and imaginary parts of $\alpha(\omega)$, which become dependent on each other. We now work out this connection, called the Kramers-Kronig relation.

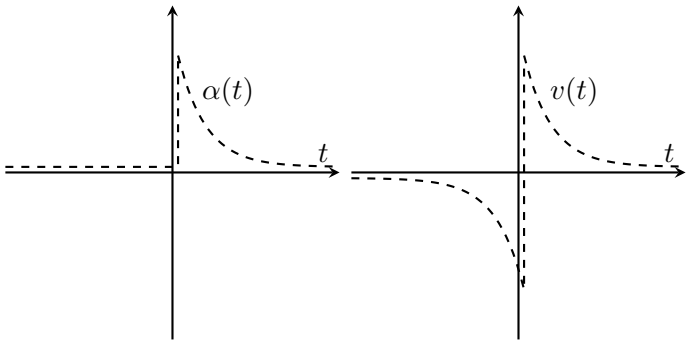

Fig. 8.3: The actual linear response function $\alpha(t)$ and its antisymmetric modification $v(t)$, introduced in Eq. (8.28).

Write $\alpha(\omega) = \alpha'(\omega) + i\alpha''(\omega)$. Now define a new function of time, $v(t)$, antisymmetric w.r.t. $t \to -t$, so that $\alpha(t) = \Theta(t)v(t)$ with $\Theta(t)$ the Heaviside step-function. Then the Fourier-transform is given by the convolution

$$\alpha(\omega) = \int_{-\infty}^{\infty} \Theta(\omega-\omega_1)v(\omega_1)\frac{\mathrm{d}\omega_1}{2\pi}. \tag{8.28}$$

Because of our choice of $v(t)$, antisymmetric in time, its Fourier image $v(\omega)$ is purely imaginary (as well as antisymmetric, $v^*(\omega) = v(-\omega) = -v(\omega)$). An efficient way to find the Fourier-transform of the step-function is:

$$\begin{aligned}\Theta(\omega) &= \int_{-\infty}^{\infty} \Theta(t)e^{i\omega t}\,\mathrm{d}t = \left(\int_0^{\infty} e^{i\omega t-\epsilon t}\,\mathrm{d}t\right)\Big|_{\epsilon\to 0} \\ &= \frac{1}{\epsilon - i\omega}\Big|_{\epsilon\to 0} = \frac{\epsilon}{\omega^2+\epsilon^2}\Big|_{\epsilon\to 0} + \frac{i\omega}{\omega^2+\epsilon^2}\Big|_{\epsilon\to 0} \\ &= \pi\delta(\omega) + \mathrm{P}\frac{i}{\omega},\end{aligned} \tag{8.29}$$

where we used the representation of the delta-function in the first term, and the second term is understood as the principal part. We can now write the Fourier-transform of the linear response function as

$$\alpha(\omega) \equiv \alpha' + i\alpha'' = \int_{-\infty}^{\infty} \left(\pi\delta(\omega-\omega_1) + \mathrm{P}\frac{i}{\omega-\omega_1}\right)v(\omega_1)\frac{\mathrm{d}\omega_1}{2\pi}. \tag{8.30}$$

Comparing imaginary parts, we see that $v(\omega) = 2i\alpha''(\omega)$ (purely imaginary as required) and hence

$$\alpha'(\omega) = \mathrm{P}\int_{-\infty}^{\infty} \frac{\alpha''(\omega_1)}{\omega_1-\omega}\frac{\mathrm{d}\omega_1}{\pi}, \tag{8.31}$$

which is the first Kramers-Kronig relation. The derivation of the second Kramers-Kronig relation is left as an exercise:[2]

$$\alpha''(\omega) = -\mathrm{P}\int_{-\infty}^{\infty} \frac{\alpha'(\omega_1)}{\omega_1 - \omega}\frac{\mathrm{d}\omega_1}{\pi}. \tag{8.32}$$

These are very general relations, based only on the causality assumption. They find applications across a wide range of scientific subjects - in dielectric studies, spectroscopy, high energy physics, etc. Note that one always finds

"Dispersion"	$\alpha'(\omega) = \alpha'(-\omega)$	even under time reversal,
"Attenuation"	$\alpha''(\omega) = -\alpha''(-\omega)$	odd under time reversal,

i.e. it is the dissipative part (attenuation) that is sensitive to the arrow of time.

[2]Hint: consider a symmetric dummy function $v(t) = v(-t)$ with its Fourier-transform purely real.

Appendix **A**

Appendix

A.1 Reminder - Some Results from the Calculus of Variations

1. Basic: To make $\int_{t_i}^{t_f} f(y, \dot{y}, t)\,\mathrm{d}t$ an extremum you must take the function y that satisfies the *Euler-Lagrange equation*

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial f}{\partial \dot{y}}\right) - \frac{\partial f}{\partial y} = 0. \tag{A.1}$$

   The function y has fixed starting and finishing points, i.e. integrate f from t_i to t_f and optimise only over functions $y(t)$ that start at a given y_i and finish at a given y_f.

2. If f depends on several functions $y_1(t), y_2(t), \cdots, y_n(t)$then the conditions for an extremum of $\int_{t_i}^{t_f} f(\mathbf{y}, \dot{\mathbf{y}}, t)\,\mathrm{d}t$ are

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial f}{\partial \dot{y}_i}\right) - \frac{\partial f}{\partial y_i} = 0, \quad i = \{1, \cdots, n\}. \tag{A.2}$$

3. If f is independent of one of the y_i, the i^{th} condition reduces to

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial f}{\partial \dot{y}_i}\right) - 0 = 0, \tag{A.3}$$

   and therefore

$$\frac{\partial f}{\partial \dot{y}_i} = \text{const.} \tag{A.4}$$

4. If $f = f(\mathbf{y}, \mathbf{y})$, i.e. if f does not depend explicitly on t, then

$$f - \sum_i \dot{y}_i \frac{\partial f}{\partial \dot{y}_i} = \text{const.} \tag{A.5}$$

5. The function $y(t)$ that makes $\int_{t_i}^{t_f} f(y, \dot{y}, t)\,\mathrm{d}t$ an extremum, when $y(t)$ has to satisfy the constraint $\int_{t_i}^{t_f} g(y, \dot{y}, t)\,\mathrm{d}t = C$, is given by

$$\left[\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial f}{\partial \dot{y}}\right) - \frac{\partial f}{\partial y}\right] + \lambda\left[\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial g}{\partial \dot{y}}\right) - \frac{\partial g}{\partial y}\right] = 0. \tag{A.6}$$

   First determine $y(t)$ for arbitrary λ; the value of λ has then to be determined from the equation of constraint and it will depend on C.

A.2 Spectral (Fourier) Analysis

The key idea for solving many complicated multi-variable dynamical problems is the Fourier representation. To illustrate this concept, which amounts to diagonalisation in the phase space of the problem, let us consider only one dimension of space (x) and a scalar field variable $f(x)$. In the case of vector or tensor functions, one simply deals with their components separately and multi-dimensional space simply requires a repetition of the analysis for each direction (assuming we remain in Cartesian coordinates). So we start with a scalar field $f(x)$, which is real (from a mathematical standpoint it does not have to be, but it is nice to be able to identify a real physical process with it) and define an interval of space $-L < x < L$ discretised into small intervals of length $a \ll L$. The infinite continuous interval corresponds to the limiting case $L \to \infty$, $a \to 0$. There are two other important limiting cases: $L \neq \infty$, but $a \to 0$, which is a finite continuous interval, and $L \neq \infty$, $a \neq 0$, which is a finite discrete lattice. We then "define"

$$f(x) = \frac{1}{2\pi} \int_{-} \infty^{\infty} \phi(q) e^{-iqx} \, \mathrm{d}q \tag{A.7}$$

$$\phi(q) = \int f(x) e^{iqx} \, \mathrm{d}x \qquad (L \to \infty, a \to 0)$$

$$f(x) = \sum_{n-=\infty}^{\infty} \phi_n e^{-i\pi n(x/L)} \tag{A.8}$$

$$\phi_n(x) = \frac{1}{2L} \int_{-L}^{L} f(x) e^{i\pi n(x/L)} \, \mathrm{d}x \qquad (L \neq \infty, a \to 0)$$

$$f_s = \sum_{n=-N/2}^{n=N/2} \phi_n e^{-i(2\pi/N)ns} \tag{A.9}$$

$$\phi_n = \frac{1}{N} \sum_{s=-L/a}^{L/a} f_s e^{i(2\pi/N)ns} \qquad (L \neq \infty, a \neq 0), \tag{A.10}$$

where $N = 2L/a$ is an integer, the index s labels lattice points in real (x) space, as does n in the reciprocal (q) space, where the discrete lattice points are separated by $\Delta q = 2\pi/(2L)$. Obviously, one or both spaces can be continuous and we should then transform the sum to an integral

$$\int f(x) \, \mathrm{d}x = \sum a \, f(x_s) = \sum_s f_s \quad \text{where} \quad f_s \equiv a \, f(x_s) \tag{A.11}$$

$$\frac{1}{2\pi} \int \phi(q) \, \mathrm{d}q = \sum \frac{\Delta q}{2\pi} \phi(q_n) = \sum_n \phi_n \quad \text{so that} \quad \phi(q_n) \equiv 2L \, \phi_n.$$

The discrete case requires periodicity:

$$f(x) = f(x + 2\pi/\Delta q) \quad \text{and} \quad \phi(q) = \phi(q + 2\pi/a). \tag{A.12}$$

It is good to know that the number of steps is universal in both spaces, $N = 2L/a = 2\pi/(a\Delta q)$

In order to operate with Fourier transformation one needs the delta-function and its discrete counterparts. Again, not going into mathematical complexities, let us assume

that the deltafunction is "defined" as the result of integration as

$$\int_{-\infty}^{\infty} e^{\pm iAx}\,\mathrm{d}x = 2\pi\delta(A). \tag{A.13}$$

Obviously, $\int \delta(x-x_0)\,\mathrm{d}x = 1$; accordingly,

$$\sum_s a\,\delta(x_s - x_{s_0}) = \sum_s \delta_{ss_0} = 1. \tag{A.14}$$

Note the different dimensionality of $\delta(x_s - x_{s0})$ and δ_{ss0} (and equally that of $f(x)$ and f_s, etc). The factor of $1/2\pi$ is purely for convenience: some authors prefer different conventions – not that it matters in the end.

Let us examine how the present convention operates on some examples. Consider a simplified energy functional in a continuous unlimited space

$$E = \int \frac{1}{2}\kappa\left(\frac{\partial u(x)}{\partial x}\right)^2 \mathrm{d}x\,. \tag{A.15}$$

We "define" a new complex function $\tilde{u}(q)$ according to the rule (A.7) and substitute it into E, in a pedestrian way:

$$\begin{aligned} E &= \int \frac{1}{2}\kappa\left(\frac{\partial}{\partial x}\int \tilde{u}(q)e^{-iqx}\frac{\mathrm{d}q}{2\pi}\right)^2 \mathrm{d}x = \iiint \frac{1}{2}\kappa(-q_1q_2)\tilde{u}(q_1)\tilde{u}(q_2)e^{-i(q_1+q_2)x}\,\mathrm{d}x\,\frac{\mathrm{d}q_1\,\mathrm{d}q_2}{(2\pi)^2} \\ &= \iint \frac{1}{2}\kappa(-q_1q_2)\tilde{u}(q_1)\tilde{u}(q_2)2\pi\delta(q_1+q_2)\frac{\mathrm{d}q_1\,\mathrm{d}q_2}{(2\pi)^2} = \int \frac{1}{2}\kappa(q_1)^2\tilde{u}(q_1)\tilde{u}(-q_1)\frac{\mathrm{d}q_1}{2\pi} \end{aligned} \tag{A.16}$$

(after the delta-function has ensured that $q_2 = -q_1$). If, and only if, the function $u(x)$ was real, then we can say on the basis of the second line of the rule (A.7) that $\tilde{u}(q) = \tilde{u}(-q)^*$, a complex conjugate. In this case the functional becomes, as you very well know,

$$E = \int \frac{1}{2}\kappa q^2|\tilde{u}(q)|^2\frac{\mathrm{d}q}{2\pi} \tag{A.17}$$

(as a mnemonic rule, every integration in the continuous reciprocal space carries a $1/2\pi$ with it).

Now let us do the same transformation for a functional defined on a finite interval of space:

$$\begin{aligned} E &= \int_{-L}^{L}\frac{1}{2}\kappa\left(\frac{\partial u(x)}{\partial x}\right)^2\mathrm{d}x = \int_{-L}^{L}\frac{1}{2}\kappa\left(\frac{\partial}{\partial x}\sum_{n=-\infty}^{\infty}\tilde{u}\left(\frac{\pi n}{L}\right)e^{-i(\pi n/L)x}\right)^2\mathrm{d}x \\ &= \int_{-L}^{L}\sum_{n_1}\sum_{n_2}\frac{1}{2}\kappa(-q_1q_2)\tilde{u}(q_1)\tilde{u}(q_2)e^{-i(q_1+q_2)x}\,\mathrm{d}x \quad \text{with discrete } q_i \equiv \frac{\pi n_i}{L} \\ &= \sum_{n_1}\sum_{n_2}\frac{1}{2}\kappa(-q_1q_2)\tilde{u}(q_1)\tilde{u}(q_2)\,2L\left[\frac{\sin\pi(n_1+n_2)}{\pi(n_1+n_2)}\right], \end{aligned} \tag{A.18}$$

where the explicit integration gave $\int_{-L}^{L} e^{-iAx}\,\mathrm{d}x = \frac{2}{A}\sin(AL)$. Because (n_1+n_2) is an integer, the sine is always equal to zero. However, if $n_1+n_2 = 0$, then the fraction is equal to one: this is a Kronecker symbol δ_{n_1,n_2}. As in the continuous integration case before, we lose one of the summations and are left with

$$E = 2L\sum_n \frac{1}{2}\kappa q_n^2|\tilde{u}(q_n)|^2, \quad q_n = \frac{\pi n}{L}. \tag{A.19}$$

As an exercise, try verifying that a convolution of functions in real space transforms into the product of their Fourier images, e.g., $\int G(y-x)u(x)v(y)\,\mathrm{d}x\,\mathrm{d}y \implies \int G(q)\tilde{u}(q)\tilde{v}(-q)\frac{\mathrm{d}q}{2\pi}$ (and the analogous summation for the finite spatial domain).

Appendix B

Appendix: Euler-Lagrange Equations

B.1 Functionals

Consider the following definite integral involving a real function $y(x)$,

$$G = \int_\alpha^\beta \left[(y'(x))^2 - (y(x))^2 \right] \mathrm{d}x \,. \tag{B.1}$$

The real number G is independent of x but depends on $y(x)$. This is a simple example of a *functional* and we denote it by $G[y]$. A real function of many variables $\{y_k; k = 1, 2, \ldots, N\}$ takes $\{y_k\}$ and gives a real number as output,

$$f : \{y_k\} \to f(\{y_k\}) \in \mathbb{R}. \tag{B.2}$$

A real functional is a generalization to a continuous infinity of variables $\{y(x); x \in \mathbb{R}\}$. It takes a function $y(x)$ and gives a real number as output,

$$G : y(x) \to G[y] \in \mathbb{R}. \tag{B.3}$$

In Eq. (B.1) above the integrand of $G[y]$ *implicitly* depends on x through y and its derivatives, but it may also *explicitly* depend on x,

$$G[y] = \int_\alpha^\beta f(y, y', y'', \cdots; x) \, \mathrm{d}x \,. \tag{B.4}$$

In general, there may be more dependent variables $\{y_i\}$ and a multiple integral over a number of independent variables $\{y_i\}$. We shall usually be concerned with functionals of the form,

$$G[y] = \int_\alpha^\beta f(y, y'; x) \, \mathrm{d}x \,. \tag{B.5}$$

The calculus of variations extends the calculus of functions to functionals It aims to answer questions such as: what functions $y(x)$ extremise the functional $G[y]$?

- It will usually be obvious from the problem whether a given extremum is a maximum, a minimum or something else – there's no equivalent of the usual criteria for functions (or at least one that's practical to use).
- We must also keep in mind that, as with ordinary calculus, an extremum we find may be only a *local* extremum and not a *global* extremum.

Functionals are useful because many problems can be formulated as a *variational principle*, the extremisation of some functional. E.g. a chain suspended between two fixed points hangs in equilibrium such that its total potential energy is minimized and an extension of this idea (incorporating chemical potential energy) can be applied to chemical reactions. An important example is *Hamilton's principle of least action* in mechanics.

B.2 Functional Derivatives

Consider the effect of changing a function $y(x)$ to a nearby function $y(x) + \delta y(x)$. The variation of G is defined by

$$\begin{aligned}\delta G &= g[y+\delta y] - G[y] \\ &= \int_\alpha^\beta f(y+\delta y, y'+(\delta y)'; x)\,\mathrm{d}x - \int_\alpha^\beta f(y, y'; x) \\ &= \int_\alpha^\beta \left[\delta y \frac{\partial f}{\partial y} + (\delta y)' \frac{\partial f}{\partial y'}\right]\mathrm{d}x + \cdots \\ &= \left[\delta y \frac{\partial f}{\partial y'}\right] + \int_\alpha^\beta \delta y \left[\frac{\partial f}{\partial y} - \frac{\mathrm{d}}{\mathrm{d}x}\left(\frac{\partial f}{\partial y'}\right)\right]\mathrm{d}x + \cdots . \end{aligned} \tag{B.6}$$

where we have omitted terms of order $(\delta y)^2$. If the boundary term is zero (e.g. if y is fixed on the boundary) then

$$\delta G = \int_\alpha^\beta \delta y(x) \frac{\delta G}{\delta y(x)}\,\mathrm{d}x + \cdots . \tag{B.7}$$

Here we have *defined* the *functional derivative* of G with respect to the function y to be,

$$\frac{\delta G}{\delta y(x)} \equiv \frac{\partial f}{\partial y} - \frac{\mathrm{d}}{\mathrm{d}x}\left(\frac{\partial f}{\partial y'}\right). \tag{B.8}$$

Note that this depends on x. (Compare with the variation of a function $f(\{y_i\})$: $\delta f = \sum_i \delta y_i \;\partial f/\partial y_i$.) The functional is stationary when $\delta G/\delta y(x) = 0$, i.e.

$$\boxed{\frac{\mathrm{d}}{\mathrm{d}x}\left(\frac{\partial f}{\partial y'}\right) = \frac{\partial f}{\partial y}.} \tag{B.9}$$

This is the **Euler-Lagrange (EL) equation**.

Note on notation: $\partial f/\partial y'$ may look strange - it seems impossible for y' to change if y doesn't. Here $\partial/\partial y$ and $\partial/\partial y'$ are just formal derivatives: pretend that y and y' are unconnected. By contrast, $\mathrm{d}/\mathrm{d}x$ is the usual full derivative with respect to x.

B.3 First Integral

In the example above we reduced the second-order EL equation to a first-order equation, $y' = const.$, a "*first integral*" of the EL equation. We found $\partial f/\partial y = 0$ and so the EL equation gave $\partial f/\partial y' = const.$ We can also reduce the EL equation to a first integral if $\partial f/\partial x = 0$, i.e. $f(y, y'; x)$ has no explicit dependence on x. Indeed, from the chain rule we have,

$$\frac{\mathrm{d}f}{\mathrm{d}x} = \frac{\partial f}{\partial x} + y'\frac{\partial f}{\partial y} + y''\frac{\partial f}{\partial y'}. \tag{B.10}$$

Using the EL equation gives,

$$\begin{aligned}\frac{\mathrm{d}f}{\mathrm{d}x} &= \frac{\partial f}{\partial x} + y'\frac{\mathrm{d}}{\mathrm{d}x}\left(\frac{\partial f}{\partial y'}\right) + y''\frac{\partial f}{\partial y'} \\ &= \frac{\partial f}{\partial x} + \frac{\mathrm{d}}{\mathrm{d}x}\left(y'\frac{\partial f}{\partial y'}\right), \end{aligned} \tag{B.11}$$

and hence

$$\frac{\mathrm{d}}{\mathrm{d}x}\left(f - y'\frac{\partial f}{\partial y'}\right) = \frac{\partial f}{\partial x}. \tag{B.12}$$

When $\partial f/\partial x = 0$,

$$\boxed{y'\frac{\partial f}{\partial y'} - f = \text{const.}} \tag{B.13}$$

B.4 Hamilton's Principle

Lagrange and Hamilton developed a powerful reformulation of Newtonian mechanics in terms of a "principle of least action" based on energy rather than force. The time evolution of a system is viewed as the motion of a point in a multi-dimensional *configuration space* described by some *generalised coordinates* $\{q_i\}$. Examples:

- A system of n particles ($3n$-dimensional coordinate space) can be described by the 3 coordinates for each of n positions.
- A rigid pendulum swinging in a vertical plane requires one generalised coordinate, the angle to the vertical.
- A top spinning on its axis on a smooth plane requires five generalised coordinates: two to describe the position of the point of contact, one for the angle of the axis to the vertical, one for the rotation of the axis about the vertical, and one for the rotation of the top about its axis.

Problems can often be simplified by a convenient choice of generalised coordinates – this is part of the power of these methods.

The *Lagrangian* is defined as

$$\boxed{\mathcal{L} = T - V} \tag{B.14}$$

where T is the kinetic energy and V is the potential energy. The action of a path, starting at time t_i and ending at t_f, is given by,

$$\boxed{S[\{q_i\}] = \int_{t_i}^{t_f} \mathcal{L}(\{q_i\}, \{\dot{q}_i\}, \cdots; t)\,\mathrm{d}t\,.} \tag{B.15}$$

Hamilton's principle states that the motion in configuration space extremises the action functional S. For $\mathcal{L}(\{q_i\}, \{\dot{q}_i\}; t)$, with N generalised coordinates and fixed start and end points,

$$\boxed{\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial \mathcal{L}}{\partial \dot{q}_i}\right) - \frac{\partial \mathcal{L}}{\partial q_i} = 0, \quad i = 1, \cdots, N.} \tag{B.16}$$

These are Lagrange's equations. If $\mathcal{L}(\{q_i\}, \{\dot{q}_i\}; t)$ has *no explicity dependence on* t, generalising the derivation of the first integral, we can find a constant of the motion. The chain rule and Lagrange's equations give,

$$\frac{\mathrm{d}\mathcal{L}}{\mathrm{d}t} = \frac{\partial \mathcal{L}}{\partial t} + \sum_{i=1}^{N}\left\{\dot{q}_i\frac{\partial \mathcal{L}}{\partial q_i} + \ddot{q}_i\frac{\partial \mathcal{L}}{\partial \dot{q}_i}\right\} = \frac{\partial \mathcal{L}}{\partial t} + \frac{\mathrm{d}}{\mathrm{d}t}\left(\sum_{i=1}^{N}\dot{q}_i\frac{\partial \mathcal{L}}{\partial \dot{q}_i}\right), \tag{B.17}$$

and hence,

$$\frac{\mathrm{d}}{\mathrm{d}t}\left[\mathcal{L} - \sum_{i=1}^{N} \dot{q}_i \frac{\partial \mathcal{L}}{\partial \dot{q}_i}\right] = \frac{\partial \mathcal{L}}{\partial t}. \tag{B.18}$$

Given $\partial \mathcal{L}/\partial t = 0$ we have,

$$\boxed{\sum_{i=1}^{N} \dot{q}_i \frac{\partial \mathcal{L}}{\partial \dot{q}_i} - \mathcal{L} = \text{const.}} \tag{B.19}$$

In general, if $\mathcal{L}$ does not explicitly depend on time, T is a homogeneous quadratic in the generalised velocities $\{\dot{q}_i\}$, i.e. $T \sim \sum_i \sum_j a_{ij}(q_1, \cdots, q_N)\dot{q}_i\dot{q}_j$, and V does not depend on $\{\dot{q}_i\}$, then it can be shown that,

$$\sum_{i=1}^{N} \dot{q}_i \frac{\partial \mathcal{L}}{\partial \dot{q}_i} - \mathcal{L} = T + V = \text{const.} \tag{B.20}$$

i.e. the total energy $E = T + V$ is conserved.

Appendix C

Appendix: Contour Integration

In this section we shall explore properties of analytic functions and functions that contain singularities. This will lead to a powerful method for doing integrals such as

$$\int_0^{2\pi} \frac{\mathrm{d}\theta}{2(a-\cos\theta)} \quad \text{and} \quad \int_0^{\infty} \frac{\mathrm{d}x}{1+x^4}. \tag{C.1}$$

C.1 Analytic Functions of a Complex Variable

C.1.1 Complex differentiability

The complex derivative of the function $f(z)$ at the point $z = z_0$ is defined as

$$f'(z_0) = \lim_{z \to z_0} \frac{f(z) - f(z_0)}{\delta z}, \tag{C.2}$$

where the same limit must be obtained for any sequence of complex values for z that tends to z_0. If this same limit exists, the function $f(z)$ is said to be **complex differentiable** at $z = z_0$.

Another way to write this is

$$\frac{\mathrm{d}f}{\mathrm{d}z} \equiv f'(z) = \lim_{\delta z \to 0} \frac{f(z+\delta z) - f(z)}{\delta z}, \tag{C.3}$$

where the limit must be the same when $\delta x \to 0$ by any route/direction in the complex plane.

Requiring a function of a *complex* variable to be differentiable is a surprisingly strong constraint.

C.1.2 The Cauchy–Riemann equations

Express $f = u + iv$ and $z = x + iy$ in terms of their real and imaginary parts,

$$f(z) = u(x, y) + iv(x, y). \tag{C.4}$$

If $f'(z)$ exists we can calculate it by assuming that $\delta z = \delta x + i\delta y$ approaches 0 along the real axis, i.e. by taking $\delta y = 0$; then

$$\begin{aligned} f'(z) &= \lim_{\delta x\to 0} \frac{f(z+\delta x) - f(z)}{\delta x} \\ &= \lim_{\delta x\to 0} \frac{u(x+\delta x, y) + iv(x+\delta x, y) - u(x,y) - iv(x,y)}{\delta x} \\ &= \lim_{\delta x\to 0} \frac{u(x+\delta x, y) - u(x,y)}{\delta x} + i \lim_{\delta x\to 0} \frac{v(x+\delta x, y) - v(x,y)}{\delta x} \\ &= \frac{\partial u}{\partial x} + i\frac{\partial v}{\partial x}. \end{aligned} \tag{C.5}$$

However, from definition (C.2), the derivative must have the same value if δz approaches 0 along the imaginary axis, i.e. by taking $\delta x = 0$; then

$$\begin{aligned} f'(z) &= \lim_{\delta y\to 0} \frac{f(z+\delta y) - f(z)}{i\delta y} \\ &= \lim_{\delta y\to 0} \frac{u(x, y+\delta y) + iv(x, y+\delta y) - u(x,y) - iv(x,y)}{i\delta y} \\ &= -i \lim_{\delta y\to 0} \frac{u(x, y+\delta y) - u(x,y)}{\delta x} + \lim_{\delta y\to 0} \frac{v(x, y+\delta y) - v(x,y)}{\delta y} \\ &= -i\frac{\partial u}{\partial y} + \frac{\partial v}{\partial y}. \end{aligned} \tag{C.6}$$

Comparing the real and imaginary parts of (C.5) and (C.6), we deduce the *Cauchy–Riemann equations*,

$$\boxed{\frac{\partial u}{\partial x} = \frac{\partial v}{\partial y}, \quad \frac{\partial v}{\partial x} = -\frac{\partial u}{\partial y}.} \tag{C.7}$$

These are necessary conditions for $f(z)$ to have a complex derivative. They are also sufficient conditions, provided that the partial derivatives are also continuous.

If we think of f as depending on z and $z^* = x - iy$ instead of x and y, the Cauchy-Riemann equations are equivalent to requiring that $\partial f/\partial z^* = 0$.

C.1.3 Analytic Functions

If a function $f(z)$ has a complex derivative at every point z in a region $\mathbf{R}$ of the complex plane, it is said to be **analytic** in $\mathbf{R}$. An *entire function* is one that is analytic in the whole complex plane.

To be analytic at a point $z = z_0$, $f(z)$ must be differentiable throughout some neighbourhood $|z - z_0| < \varepsilon$ of that point.

Many complex functions are analytic everywhere in the complex plane except at isolated points, which are called the *singular points* or *singularities* of the function.

C.1.4 Consequences of the Cauchy–Riemann equations

If we know the real part of an analytic function in some region, we can find its imaginary part (or vice versa) up to an additive constant by integrating the Cauchy–Riemann equations.

The real and imaginary parts of an analytic function satisfy Laplace's equation (they are harmonic functions),

$$\begin{aligned}\frac{\partial^2 u}{\partial x^2}+\frac{\partial^2 u}{\partial y^2} &= \frac{\partial}{\partial x}\left(\frac{\partial u}{\partial x}\right)+\frac{\partial}{\partial y}\left(\frac{\partial u}{\partial y}\right)\\ &= \frac{\partial}{\partial x}\left(\frac{\partial v}{\partial y}\right)+\frac{\partial}{\partial y}\left(-\frac{\partial v}{\partial x}\right)\\ &= 0.\end{aligned} \tag{C.8}$$

The proof that $\nabla^2 v = 0$ is similar.

This property provides a useful method for solving Laplace's equation in two dimensions: one "just" needs to find an analytic function that satisfies the boundary conditions.

Using the Cauchy–Riemann equations (C.7), we see that

$$\begin{aligned}\boldsymbol{\nabla} u\cdot\boldsymbol{\nabla} v &= \frac{\partial u}{\partial x}\frac{\partial v}{\partial x}+\frac{\partial u}{\partial y}\frac{\partial v}{\partial y}\\ &= \frac{\partial v}{\partial y}\frac{\partial v}{\partial x}-\frac{\partial v}{\partial x}\frac{\partial v}{\partial y}\\ &= 0.\end{aligned} \tag{C.9}$$

Hence the curves of constant u and those of constant v are orthogonal: u and v are said to be *conjugate harmonic functions*.

C.1.5 Taylor series for analytic functions

If a function of a complex variable is analytic in a region $\mathbf{R}$ of the complex plane, not only is it differentiable everywhere in $\mathbf{R}$, it is also differentiable any number of times. It follows that if $f(z)$ is analytic at $z = z_0$, it has an infinite Taylor series

$$f(z)=\sum_{n=0}^{\infty} a_n (z-z_0)^n \quad \text{where} \quad a_n = \frac{1}{n!}f^{(n)}(z_0) \equiv \frac{1}{n!}\frac{\mathrm{d}^2 f}{\mathrm{d}z^2}. \tag{C.10}$$

This series converges within some neighbourhood of z_0.

An alternative definition of the analyticity of a function $f(z)$ at $z = z_0$ is that $f(z)$ has a Taylor series expansion about $z = z_0$ with a *non-zero radius of convergence*.

C.2 Zeros, Poles and Essential Singularities

C.2.1 Zeros of Complex Functions

The zeros of $f(z)$ are the points $z = z_0$ in the complex plane where $f(z_0) = 0$. A zero is of **order** N if

$$f(z_0) = f'(z_0) = f''(z_0) = \cdots = f^{(N-1)}(z_0) = 0 \quad \text{but} \quad f^{(N)}(z_0) \neq 0. \tag{C.11}$$

The first non-zero term in the Taylor series of $f(z)$ about $z = z_0$ is then proportional to $(z - z_0)^N$. Indeed

$$f(z) \sim a_N (z - z_0)^N \quad \text{as} \quad z \to z_0. \tag{C.12}$$

A *simple zero* is a zero of order 1. A *double zero* is one of order 2, etc.

C.2.2 Poles of Complex Functions

Suppose $g(z)$ is analytic and non-zero at $z = z_0$. Consider the function

$$f(z) = (z - z_0)^{-N} g(z), \tag{C.13}$$

in which case

$$f(z) \sim g(z_0)(z - z_0)^{-N} \quad \text{as} \quad z \to z_0. \tag{C.14}$$

$f(z)$ is not analytic at $z = z_0$, and we say that $f(z)$ has a *pole of order* N. We refer to a pole of order 1 as a *simple pole*, a pole of order 2 as a *double pole*, etc.

Because $g(z)$ is analytic, from (C.10) it has a Taylor series expansion at z_0,

$$g(z) = \sum_{n=0}^{\infty} b_n (z - z_0)^n \quad \text{with} \quad b_0 \neq 0. \tag{C.15}$$

Hence,

$$f(z) = (z - z_0)^{-N} g(z) = \sum_{n=-N}^{\infty} a_n (z - z_0)^n, \tag{C.16}$$

with $a_n = b_{n+N}$, and $a_{-N} \neq 0$. This is not a Taylor series because it includes negative powers of $z - z_0$, and $f(z)$ is not analytic at $z = z_0$.

If $f(z)$ has a zero of order N at $z = z_0$, then $1/f(z)$ has a pole of order N there, and vice versa.

If $f(z)$ is analytic and non-zero at $z = z_0$ and $g(z)$ has a zero of order N there, then $f(z)/g(z)$ has a pole of order N there.

C.2.3 Laurent Series and Essential Singularities

It can be shown that any function that is analytic (and single-valued) throughout an annulus $\alpha < |z - z_0| < \beta$ centred on a point $z = z_0$ has a unique *Laurent series*,

$$f(z) = \sum_{n=-\infty}^{\infty} a_n (z - z_0)^n, \tag{C.17}$$

which converges for all values of z within the annulus.

If $\alpha = 0$, then $f(z)$ is analytic throughout the disk $|z - z_0| < \beta$ except possibly at $z = z_0$ itself, and the Laurent series determines the behaviour of $f(z)$ near $z = z_0$. There are three possibilities:

1. If the first non-zero term in the Laurent series has $n \geq 0$, then $f(z)$ is analytic at $z = z_0$ and the series is just a Taylor series;
2. If the first non-zero term in the Laurent series has $n = -N < 0$, then $f(z)$ has a pole of order N at $z = z_0$;
3. Otherwise, if the Laurent series involves an infinite number of terms with $n < 0$, then $f(z)$ has an *essential singularity* at $z = z_0$.

The behaviour of a function near an essential singularity is remarkably complicated. *Picard's theorem* states that, in any neighbourhood of an essential singularity, the function takes all possible complex values (possibly with one exception) at infinitely many points.

C.3 Contour integrals

Consider an integral $\int_{\mathcal{C}} f(z)\,\mathrm{d}z$ from $z = a$ to b in the complex plane. We need to specify the path or contour, $\mathcal{C}$, along which we integrate. For example, consider the integral $\int \frac{1}{z}\,\mathrm{d}z$ from $z = -1$ to $z = +1$ along paths around half the unit circle (1) clockwise (above the real axis) and (2) anticlockwise (below the real axis).

Making the substitution $z = e^{i\theta}$, $\mathrm{d}z = ie^{i\theta}\,\mathrm{d}\theta$,

$$I_1 = \int_{\pi}^{0} \frac{ie^{i\theta}}{e^{i\theta}}\,\mathrm{d}\theta = \int_{\pi}^{0} i\,\mathrm{d}\theta = -i\pi, \tag{C.18}$$

and

$$I_2 = \int_{\pi}^{2\pi} i\,\mathrm{d}\theta = +i\pi. \tag{C.19}$$

Therefore, the *result of a contour integration may depend on the contour.*

The integral can be formally defined by dividing $\mathcal{C}$ into small intervals $\delta z_k = z_{k+1} - z_k$, where $k = 0, \cdots, N$; $z_0 = a$ and $z_N = b$. Then we define,

$$\int_{\mathcal{C}} f(z)\,\mathrm{d}z = \lim_{\Delta \to 0} \sum_{k=0}^{N-1} f(z_k)\delta z_k, \tag{C.20}$$

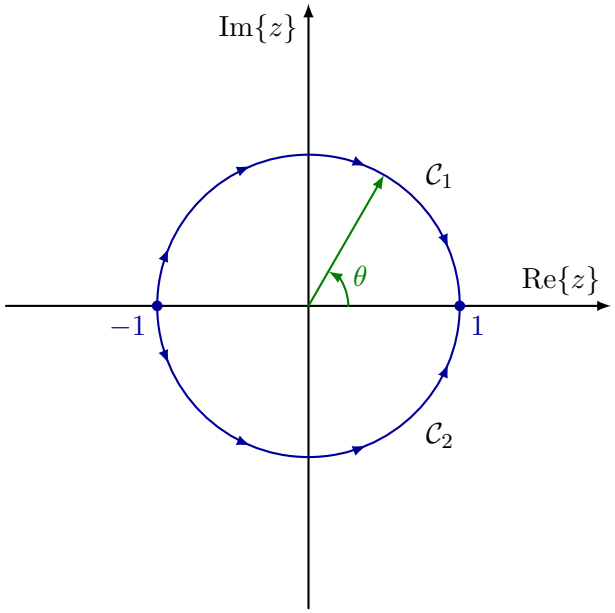

Fig. C.1: The paths for contour integration around half the unit circle, $\mathcal{C}_1$ clockwise (above the real axis) and $\mathcal{C}_2$ anticlockwise (below the real axis).

where $\Delta = \max_k |\delta z_k|$ and $N \to \infty$ as $\Delta \to 0$. The following properties follow from this definition:

- If $\mathcal{C}_1$ is a contour from a to b, $\mathcal{C}_2$ is a contour from b to c, and $\mathcal{C}$ is $\mathcal{C}_1$ followed by $\mathcal{C}_2$, then
$$\int_{\mathcal{C}} f(z)\,\mathrm{d}z = \int_{\mathcal{C}_1} f(z)\,\mathrm{d}z + \int_{\mathcal{C}_2} f(z)\,\mathrm{d}z\,. \tag{C.21}$$
- If $\mathcal{C}_+$ is a contour from a to b and $\mathcal{C}_-$ is the contour in reverse,
$$\int_{\mathcal{C}_+} f(z)\,\mathrm{d}z = -\int_{\mathcal{C}_-} f(z)\,\mathrm{d}z\,. \tag{C.22}$$
- We can use integration by parts and substitution.
- If the contour has length L then,
$$\left|\int_{\mathcal{C}} f(z)\,\mathrm{d}z\right| \leq L \max_{\mathcal{C}} |f(z)|. \tag{C.23}$$
- If $\mathcal{C}$ is a closed contour then it doesn't matter where we start on $\mathcal{C}$. However, if we reverse the direction of $\mathcal{C}$ the integral changes sign,
$$\oint_{\text{anticlockwise}} f(z)\,\mathrm{d}z = -\oint_{\text{clockwise}} f(z)\,\mathrm{d}z\,. \tag{C.24}$$
We can again split the integral up into two parts,
$$\int_{\mathcal{C}} f(z)\,\mathrm{d}z = \int_{\mathcal{C}_1} f(z)\,\mathrm{d}z + \int_{\mathcal{C}_2} f(z)\,\mathrm{d}z\,. \tag{C.25}$$

C.4 Cauchy's theorem

A *simply-connected domain* is a region **R** of the complex plane without any holes; any closed curve in **R** encircles points which are only in **R**. A *simple closed curve* is a continuous closed curve of finite length that does not intersect itself; it divides the complex plane into an interior region and an exterior region.

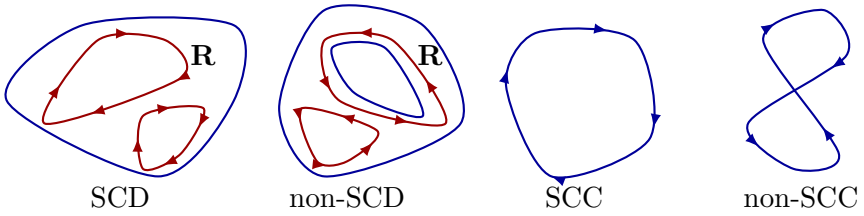

Fig. C.2: A simply-connected domain **R** is a region without holes; any closed curve encircles points only in **R**. A simple closed curve is a continuous closed curve of finite length that does not intersect itself.

Cauchy's theorem states that if a function $f(z)$ is analytic in a simply-connected domain **R**, then for any simple closed curve $\mathcal{C}$ in **R**,

$$\boxed{\oint_{\mathcal{C}} f(z)\,\mathrm{d}z = 0.} \tag{C.26}$$

In the proof we'll need a 2D version of the divergence theorem (Green's theorem in a plane). We first introduce a 3D vector field $\mathbf{A} = (A_x, A_y, 0) = (-a_y, a_x, 0)$ and integrate the curl of $\mathbf{A}$ over the surface $\mathcal{S}$ inside the simple closed curve $\mathcal{C}$, imagining it existing inside the 2D plane $z = 0$,

$$\int_{\mathcal{S}} (\boldsymbol{\nabla} \times \mathbf{A}) \cdot \mathrm{d}\mathbf{S} = \int_{\mathcal{S}} \left(\frac{\partial A_y}{\partial x} - \frac{\partial A_x}{\partial y} \right) \mathrm{d}S = \int_{\mathcal{S}} \left(\frac{\partial a_x}{\partial x} + \frac{\partial a_y}{\partial y} \right) \mathrm{d}x\,\mathrm{d}y\,. \tag{C.27}$$

Now consider the line integral of $\mathbf{A}$ along $\mathcal{C}$,

$$\oint_{\mathcal{C}} \mathbf{A} \cdot \mathrm{d}\mathbf{l} = \oint_{\mathcal{C}} (A_x\,\mathrm{d}x + A_y\,\mathrm{d}y) = \oint_{\mathcal{C}} (a_x\,\mathrm{d}y - a_y\,\mathrm{d}x). \tag{C.28}$$

Thus invoking the 3D divergence theorem we arrive at

$$\int_{\mathcal{S}} \left(\frac{\partial a_x}{\partial x} + \frac{\partial a_y}{\partial y} \right) \mathrm{d}x\,\mathrm{d}y = \oint_{\mathcal{C}} (a_x\,\mathrm{d}y - a_y\,\mathrm{d}x). \tag{C.29}$$

Using this, writing f and z as real and imaginary parts, and using the Cauchy-Riemann equations (C.7) (f is analytic throughout $\mathcal{S}$),

$$\begin{aligned}
\oint_{\mathcal{C}} f(z)\,\mathrm{d}z &= \oint_{\mathcal{C}} (u + iv)(\mathrm{d}x + i\,\mathrm{d}y) \\
&= \oint_{\mathcal{C}} (u\,\mathrm{d}x - v\,\mathrm{d}y) + i \oint_{\mathcal{C}} (v\,\mathrm{d}x + u\,\mathrm{d}y) \\
&= \int_{\mathcal{S}} \underbrace{\left(-\frac{\partial v}{\partial x} - \frac{\partial u}{\partial y} \right)}_{=0} \mathrm{d}x\,\mathrm{d}y + i \int_{\mathcal{S}} \underbrace{\left(\frac{\partial u}{\partial x} - \frac{\partial v}{\partial y} \right)}_{=0} \mathrm{d}x\,\mathrm{d}y \\
&= 0.
\end{aligned} \tag{C.30}$$

C.4.1 Deforming Contours

Using Cauchy's theorem, we deduce that if we have two different contours, $\mathcal{C}_1$ and $\mathcal{C}_2$, from a to b, then, if there are no singularities between them,

$$\oint_{\mathcal{C}} f(z)\,\mathrm{d}z = \int_{\mathcal{C}_1} f(z)\,\mathrm{d}z - \int_{\mathcal{C}_2} f(z)\,\mathrm{d}z = 0, \tag{C.31}$$

and so

$$\int_{\mathcal{C}_1} f(z)\,\mathrm{d}z = \int_{\mathcal{C}_2} f(z)\,\mathrm{d}z = 0. \tag{C.32}$$

Therefore, we can deform a contour without changing the value of the integral as long as we don't move the contour across a singularity.

We can deform a closed contour, without passing it through any singularities to find that, because the joins cancel,

$$\oint_{\mathcal{C}} f(z)\,\mathrm{d}z = \oint_{\mathcal{C}_1} f(z)\,\mathrm{d}z - \oint_{\mathcal{C}_2} f(z)\,\mathrm{d}z = 0 \quad \Longrightarrow \quad \oint_{\mathcal{C}_1} f(z)\,\mathrm{d}z = \oint_{\mathcal{C}_2} f(z)\,\mathrm{d}z\,. \tag{C.33}$$

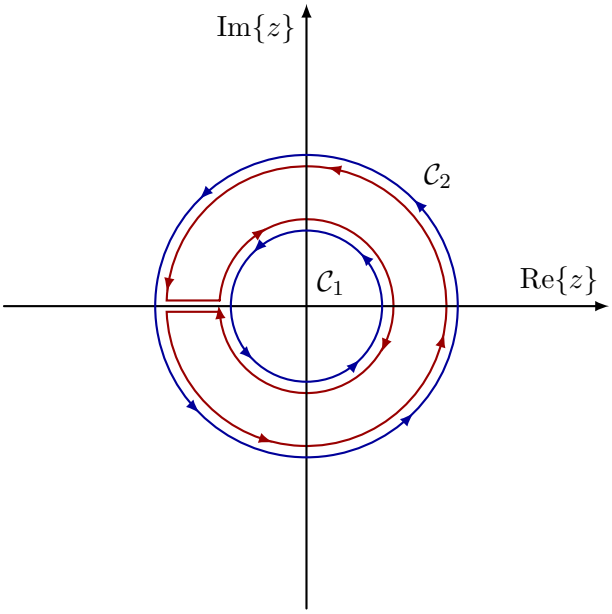

Fig. C.3: We can deform a contour without changing the value of the integral as long as we don't move the contour across a singularity.

If f and f' are analytic in some simply-connected domain $\mathbf{R}$ then,

$$\int_a^b f'(z)\,\mathrm{d}z = \int_0^1 f'(z(s))\frac{\mathrm{d}z}{\mathrm{d}s}\,\mathrm{d}s = \int_0^1 \frac{\mathrm{d}f(z(s))}{\mathrm{d}s}\,\mathrm{d}s = [f(z(s))]_0^1, \tag{C.34}$$

implying

$$\boxed{\int_a^b f'(z)\,\mathrm{d}z = f(b) - f(a),} \tag{C.35}$$

where a, b and the integration contour lie in $\mathbf{R}$. In this case integration is the inverse of differentiation in the same sense as for real functions of a real variable.

Note that if f is analytic at z_0 it can be written as g' for some other function g that is analytic at z_0.

If f has no singularities anywhere then the integral $\int_a^b f(z)\,\mathrm{d}z$ does not depend at all on the path taken.

Cauchy's theorem does *not* hold if there is a singularity inside $\mathcal{C}$ [$f(z)$ is then not analytic in $\mathbf{R}$]. For the example of $f(z) = 1/z$, if $\mathcal{C}$ is a contour anticlockwise around the unit circle,

$$\oint_{\mathcal{C}} f(z)\,\mathrm{d}z = \int_{\mathcal{C}_2} \frac{1}{z}\,\mathrm{d}z - \int_{\mathcal{C}_1} \frac{1}{z}\,\mathrm{d}z = i\int_0^{2\pi} \mathrm{d}\theta = 2\pi i \neq 0. \tag{C.36}$$

In this case $f(z)$ has a singularity, a simple pole, at $z = 0$.

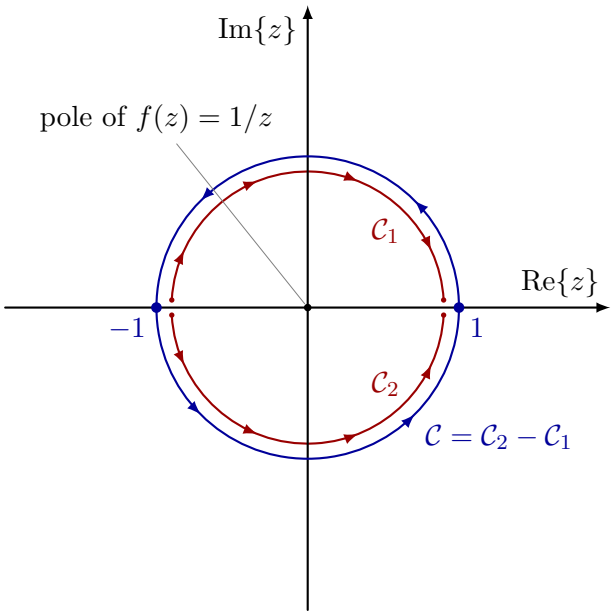

Fig. C.4: Cauchy's theorem does not hold if there is a singularity inside $\mathcal{C}$. For the example of $f(z) = 1/z$, if $\mathcal{C}$ is a contour anticlockwise around the unit circle, $\oint_{\mathcal{C}} f(z)\,\mathrm{d}z \neq 0$. In this case $f(z)$ has a singularity, a simple pole, at $z = 0$.

C.5 Residues

It can be shown that any function, which is analytic and single-valued throughout an annulus $a < |z - z_0| < b$ centred on $z = z_0$, has a unique **Laurent series** (C.17) about $z = z_0$,

$$f(z) = \sum_{n=-\infty}^{\infty} a_n (z - z_0)^n, \tag{C.37}$$

which converges for all values of z within the annulus.

If $f(z)$ has a single isolated singularity at $z = z_0$ then $a > 0$ can be made arbitrarily small. In this case, if $a_{-n} = 0$ for $n > N$ but $a_{-N} \neq 0$ then $f(z)$ has a *pole of order* N at z'. If there is no such N (i.e. the expansion in negative powers of $z - z_0$ does not terminate) the point z_0 is an essential singularity (See Section C.2).

For a general $f(z)$ with a pole of order N,

$$f(z) = \frac{a_{-N}}{(z-z_0)^N} + \frac{a_{-N+1}}{(z-z_0)^{N-1}} + \cdots + \frac{a_{-1}}{z-z_0} + a_0 + a_1(z-z_0) + \cdots , \tag{C.38}$$

The coefficient a_{-1} is called the **residue** of the pole. For a simple pole,

$$\operatorname*{res}_{z=z_0} f(z) = a_{-1} = \lim_{z\to z_0} \{(z-z_0)f(z)\}. \tag{C.39}$$

For a pole of order N,

$$\boxed{\operatorname*{res}_{z=z_0} f(z) = \lim_{z\to z_0} \left\{ \frac{1}{(N-1)!} \frac{\mathrm{d}^{N-1}}{\mathrm{d}z^{N-1}} \Big[(z-z_0)^N f(z) \Big] \right\}.} \tag{C.40}$$

as we can easily verify,

$$\begin{aligned}
\operatorname*{res}_{z=z_0} f(z) &= \lim_{z\to z_0} \left\{ \frac{1}{(N-1)!} \frac{\mathrm{d}^{N-1}}{\mathrm{d}z^{N-1}} \Big[(z-z_0)^N f(z) \Big] \right\} \\
&= \lim_{z\to z_0} \left\{ \frac{1}{(N-1)!} \frac{\mathrm{d}^{N-1}}{\mathrm{d}z^{N-1}} \Big[a_{-N} + a_{-N+1}(z-z_0) + \cdots + a_{-1}(z-z_0)^{N-1} + \cdots \Big] \right\} \\
&= \lim_{z\to z_0} \left\{ \frac{1}{(N-1)!} \Big[(N-1)!a_{-1} + N!a_0(z-z_0) + \cdots \Big] \right\} \\
&= a_{-1},
\end{aligned} \tag{C.41}$$

however for low order poles this formula luckily becomes significantly simpler to calculate.

C.6 Calculus of Residues

Consider the integral of a function, $\oint_{\mathcal{C}} f(z)\,\mathrm{d}z$, anticlockwise around a pole at $z = z_0$ where $\mathcal{C}$ lies in the region for which the Laurent series converges.

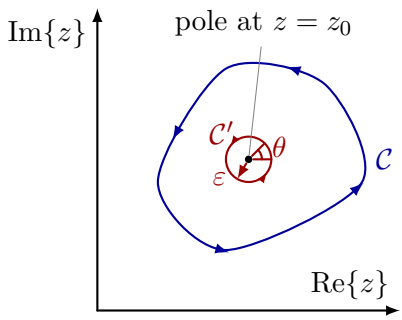

Fig. C.5: Shrinking the contour $\mathcal{C}$ to a circle of radius ε about z_0 and substituting $z = z_0 + \varepsilon e^{i\theta}$.

Considering each term of the Laurent series separately, for $n \geq 0$ the terms are analytic,

$$\oint_{\mathcal{C}} a_n (z - z_0)^n \, \mathrm{d}z = 0, \tag{C.42}$$

from Cauchy's theorem. For $n < 0$, shrink the contour to a circle of radius ε about z_0 and substitute $z = z_0 + \varepsilon e^{i\theta}$,

$$\begin{aligned}
\oint_{\mathcal{C}'} a_n (z - z_0)^n \, \mathrm{d}z &= a_n \int_0^{2\pi} \varepsilon^n e^{in\theta} i\varepsilon e^{i\theta} \, \mathrm{d}\theta \\
&= i a_n \varepsilon^{n+1} \int_0^{2\pi} e^{i(n+1)\theta} \, \mathrm{d}\theta \\
&= \begin{cases} i a_n \varepsilon^{n+1} 2\pi & n = -1 \\ i a_n \varepsilon^{n+1} \left[\dfrac{e^{i(n+1)\theta}}{i(n+1)} \right]_0^{2\pi} & n \neq 1 \end{cases} \\
&= \begin{cases} 2\pi i a_{-1} & n = -1 \\ 0 & n \neq -1 \end{cases}.
\end{aligned} \tag{C.43}$$

Therefore,

$$\begin{aligned}
\oint_{\mathcal{C}} f(z) \, \mathrm{d}z &= \sum_{n=-\infty}^{\infty} \oint_{\mathcal{C}} a_n (z - z_0)^n \, \mathrm{d}z \\
&= 2\pi i a_{-1} \\
&= 2\pi i \operatorname*{res}_{z=z_0} f(z).
\end{aligned} \tag{C.44}$$

This result leads to the **residue theorem**: if a function $f(z)$ is analytic in a simply-connected region $\mathbf{R}$ except for a finite number of poles at $z = z_1, z_2, \cdots, z_n$, and a simple closed curve $\mathcal{C}$ encircles the poles in an *anticlockwise* direction,

$$\boxed{\oint_{\mathcal{C}} f(z) \, \mathrm{d}z = 2\pi i \sum_{k=1}^{n} \operatorname*{res}_{z=z_k} f(z).} \tag{C.45}$$

To prove this, consider a new contour $\mathcal{C}'$ as shown. $\mathcal{C}'$ doesn't encircle any poles and so $\oint_{\mathcal{C}'} f(z) \, \mathrm{d}z = 0$. We can express this integral as the sum of the integral around $\mathcal{C}$ and integrals encircling each of the poles *clockwise*, $\mathcal{C}'$,

$$0 = \oint_{\mathcal{C}'} f(z) \, \mathrm{d}z = \oint_{\mathcal{C}} f(z) \, \mathrm{d}z + \sum_k \oint_{\mathcal{C}_k} f(z) \, \mathrm{d}z \, . \tag{C.46}$$

The joining lines give zero net contribution because the contribution going one way cancels with the contribution from going back. Using the result we derived for a contour encircling a single pole,

$$0 = \oint_{\mathcal{C}'} f(z) \, \mathrm{d}z = \oint_{\mathcal{C}} f(z) \, \mathrm{d}z + 2\pi i \sum_k \operatorname*{res}_{z=z_k} f(z), \tag{C.47}$$

and the residue theorem follows.

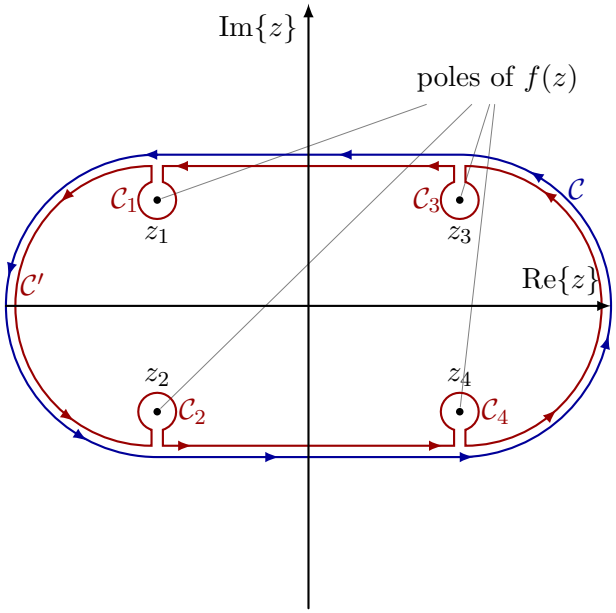

Fig. C.6: For analytic $f(z)$ in a region $\mathbf{R}$ except for a finite number of poles, a simple closed curve $\mathcal{C}$ encircling the poles in an *anticlockwise* direction has a contour integral given by the residue theorem. This can be shown by expressing this integral as the sum of the integral around $\mathcal{C}$ and integrals encircling each of the poles *clockwise*.

C.7 Cauchy's formula for $f(z)$

If $f(z)$ is analytic in a region $\mathbf{R}$ containing z_0 then **Cauchy's formula** states that,

$$\boxed{f(z_0) = \frac{1}{2\pi i} \oint_{\mathcal{C}} \frac{f(z)}{z - z_0}\, \mathrm{d}z\,,} \tag{C.48}$$

where $\mathcal{C}$ is a simple closed contour in $\mathbf{R}$ encircling z_0 anticlockwise. The proof follows immediately from the residue theorem: $f(z)/(z - z_0)$ is analytic except for a simple pole at $z = z_0$ and the residue at this pole is $f(z_0)$.

$$\oint_{\mathcal{C}} \frac{f(z)}{z - z_0}\, \mathrm{d}z = 2\pi i \times \operatorname*{res}_{z=z_0} \frac{f(z)}{z - z_0} = 2\pi i \times \lim_{z=z_0} f(z) = 2\pi i f(z_0). \tag{C.49}$$

Note: if we know $f(z)$ on $\mathcal{C}$ then, from Cauchy's formula, we know $f(z)$ throughout the interior of $\mathcal{C}$. Compare this with the uniqueness theorem for solutions of Laplace's equation with Dirichlet boundary conditions. The real and imaginary parts, u and v, of an analytic function satisfy Laplace's equation. Therefore, if we specify u and v on $\mathcal{C}$, there is a unique solution for u and v inside $\mathcal{C}$.

If we differentiate Cauchy's formula n times with respect to z_0 we obtain

$$f^{(n)}(z_0) = \frac{n!}{2\pi i} \oint_{\mathcal{C}} \frac{f(z)}{(z - z_0)^{n+1}}\, \mathrm{d}z\,. \tag{C.50}$$

Therefore, at any point where f is analytic, all its derivatives exist and it is differentiable infinitely many times.

C.8 Applications of the Calculus of Residues

We now consider some examples of using residue calculus.

Example Calculate the integral,

$$I = \int_0^{2\pi} \frac{\mathrm{d}\theta}{2(a - \cos\theta)}, \quad a > 1 \text{ is a real constant.} \tag{C.51}$$

Substitute $z = e^{i\theta}$ which gives $\mathrm{d}z = iz\,\mathrm{d}\theta$ and $\cos\theta = \frac{1}{2}(z + z^{-1})$. The integral between $\theta = 0$ and 2π is the integral over z around a circle $\mathcal{C}$ of radius 1 in the complex plane.

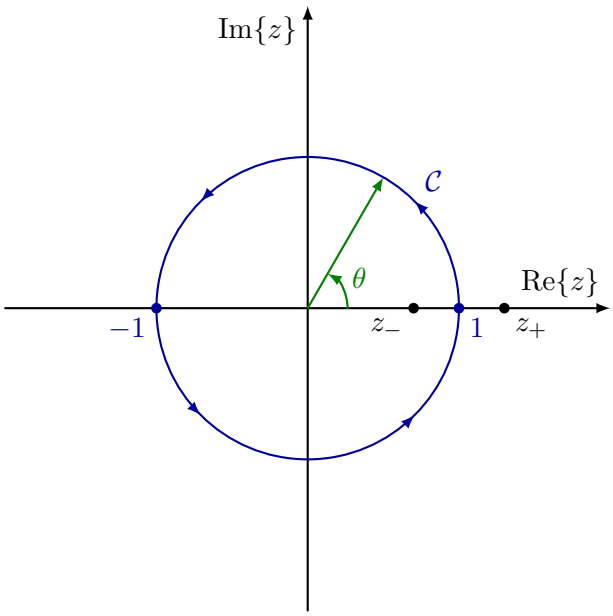

Fig. C.7: The contour $\mathcal{C}$ used for evaluating (C.51), a circle of radius 1 in the complex plane. One of the simple poles of the integral, z_-, lies within $\mathcal{C}$, but z_+ is outside it.

$$I = \oint_{\mathcal{C}} \frac{(iz)^{-1}\,\mathrm{d}z}{2\left[a - \frac{1}{2}(z + z^{-1})\right]} = +i \oint_{\mathcal{C}} \frac{\mathrm{d}z}{z^2 - 2az + 1} = +i \oint_{\mathcal{C}} \frac{\mathrm{d}z}{(z - z_+)(z - z_-)}. \tag{C.52}$$

The integrand has simple poles at $z_\pm = a \pm \sqrt{a^2 - 1}$. Because $a > 1$ the pole at z_- is inside $\mathcal{C}$ but z_+ is outside it. The residue at z_- is,

$$\frac{i}{z_- - z_+} = -\frac{i}{2\sqrt{a^2 - 1}}. \tag{C.53}$$

Therefore, from the residue theorem,

$$I = \frac{\pi}{\sqrt{a^2 - 1}}. \tag{C.54}$$

Example Calculate the integral,

$$I = \int_0^{\infty} \frac{\mathrm{d}x}{1 + x^2}. \tag{C.55}$$

We already know how to do this using trig. substitutions, but let's see how to compute it using residue calculus.

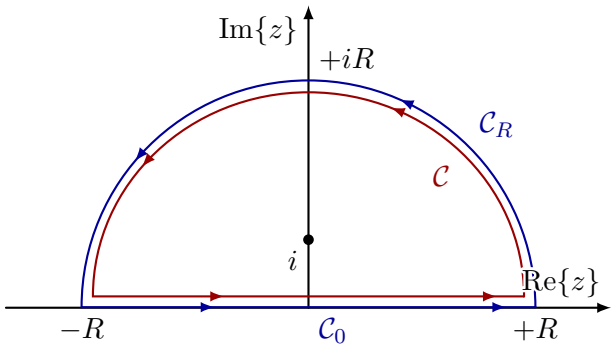

Fig. C.8: The contour $\mathcal{C}$, used to compute (C.55), is as shown a contour from $-R$ to $+R$ along the real axis ($\mathcal{C}_0$) and then along a semicircle of radius R in the upper half-plane ($\mathcal{C}_R$). The integrand has two simple poles, but only the one at $z = +i$ is enclosed by $\mathcal{C}$.

Consider,

$$\oint_{\mathcal{C}} \frac{\mathrm{d}z}{1+z^2} = \oint_{\mathcal{C}} \frac{\mathrm{d}z}{(z+i)(z-i)}, \tag{C.56}$$

where $\mathcal{C}$ is as shown a contour from $-R$ to $+R$ along the real axis ($\mathcal{C}_0$) and then along a semicircle of radius R in the upper half-plane ($\mathcal{C}_R$). The integrand has two simple poles, but only the one at $z = i$ is enclosed by $\mathcal{C}$ and so,

$$\oint_{\mathcal{C}} \frac{\mathrm{d}z}{1+z^2} = 2\pi i \frac{1}{2i} = \pi. \tag{C.57}$$

We also have,

$$\oint_{\mathcal{C}_0} \frac{\mathrm{d}z}{1+z^2} = \int_{-R}^{R} \frac{\mathrm{d}z}{1+z^2} \to 2I \quad \text{as} \quad R \to \infty. \tag{C.58}$$

What about the integral along $\mathcal{C}_R$? The integrand is $\mathcal{O}(R^{-2})$ on the semicircle and the contour has length πR. Hence,

$$\left| \int_{\mathcal{C}_R} \frac{\mathrm{d}z}{1+z^2} \right| \leq \pi R \times \mathcal{O}\left(R^{-2}\right) = \mathcal{O}\left(R^{-1}\right) \to 0 \quad \text{as} \quad R \to \infty. \tag{C.59}$$

Combining these results and taking the limit $R \to \infty$,

$$I = \frac{\pi}{2}. \tag{C.60}$$

Example Calculate the integral,

$$I = \int_0^{\infty} \frac{\mathrm{d}x}{(x^2+a^2)^2}, \quad a > 1 \text{ is a real constant.} \tag{C.61}$$

The analysis is very similar to the previous example. Consider,

$$\oint_{\mathcal{C}} \frac{\mathrm{d}x}{(x^2+a^2)^2} = \oint_{\mathcal{C}} \frac{\mathrm{d}z}{(z+ia)^2(z-ia)^2}. \tag{C.62}$$

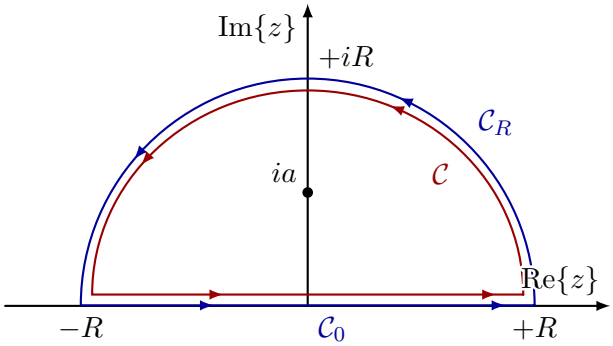

Fig. C.9: The contour $\mathcal{C}$, used to compute (C.61), is as shown a contour from $-R$ to $+R$ along the real axis ($\mathcal{C}_0$) and then along a semicircle of radius R in the upper half-plane ($\mathcal{C}_R$). The integrand has two double poles, but only the one at $z = +ia$ is enclosed by $\mathcal{C}$.

The integrand has double poles at $z = \pm ia$ but the contour only encloses the pole at $z = +ia$. The residue there is

$$\lim_{z\to+ia} \frac{\mathrm{d}}{\mathrm{d}z} \frac{1}{(z+ia)^2} = \lim_{z\to+ia} \frac{-2}{(z+ia)^3} = -\frac{1}{4} ia^{-3}. \tag{C.63}$$

The integral around the semicircle $\to 0$ as $R \to \infty$,

$$\left| \int_{\mathcal{C}_R} \frac{\mathrm{d}z}{(z^2+a^2)^2} \right| \leq \pi R \times \mathcal{O}\Big(R^{-4}\Big) = \mathcal{O}\Big(R^{-3}\Big) \to 0 \quad \text{as} \quad R \to \infty. \tag{C.64}$$

Therefore,

$$2I = 2\pi i \left(-\frac{1}{4} ia^{-3} \right) \quad \Longrightarrow \; I = \frac{\pi}{4a^3}. \tag{C.65}$$

Example Calculate the integral,

$$I = \int_0^\infty \frac{\mathrm{d}x}{1+x^4}. \tag{C.66}$$

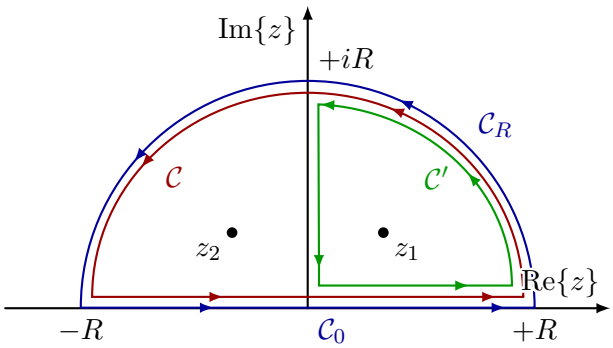

Fig. C.10: Caption

We again use a similar analysis. Consider,

$$\oint_{\mathcal{C}} \frac{\mathrm{d}x}{1+x^4} = \oint_{\mathcal{C}} \frac{\mathrm{d}z}{(z-z_1)(z-z_2)(z-z_3)(z-z_4)}, \tag{C.67}$$

where the integrand has simple poles at $z_1 = e^{\pi i/4}$, $z_2 = e^{3\pi i/4}$, $z_3 = e^{-\pi i/4}$ and $z_4 = e^{-3\pi i/4}$. Two poles, at z_1 and z_2, are enclosed by $\mathcal{C}$ with residues $-\frac{1}{4}e^{\pi i/4}$ and $\frac{1}{4}e^{-\pi i/4}$ respectively.

Therefore,

$$2I = 2\pi i\left(-\frac{1}{4}e^{\pi i/4} + \frac{1}{4}e^{-\pi i/4}\right) = \pi \sin\frac{\pi}{4} \quad \Longrightarrow \quad I = \frac{\pi}{2\sqrt{2}}. \tag{C.68}$$

Alternatively, we could use the contour $\mathcal{C}'$ enclosing quarter of a circle and so only the pole at z_1. The integral along the real axis from 0 to R, $\mathcal{C}_1 \to I$ as $R \to \infty$. The integral along $\mathcal{C}_2$ is, substituting $z = iy$,

$$\int_{\mathcal{C}_2} \frac{\mathrm{d}z}{1+z^4} = \int_R^0 \frac{i\,\mathrm{d}y}{1+y^4} = -i\int_0^R \frac{\mathrm{d}y}{1+y^4} \to -iI \quad \text{as} \quad R \to \infty. \tag{C.69}$$

The integral along $\mathcal{C}_R \to 0$ as $R \to \infty$ and so,

$$I - iI = 2\pi i\left(-\frac{1}{4}e^{\pi i/4}\right) \quad \Longrightarrow \quad I = \frac{\pi}{2\sqrt{2}}. \tag{C.70}$$

C.9 Multi-Valued Functions and Branch Cuts