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Classical field dynamics

A field is a dynamically changing potential $V(\mathbf{x}, t)$, which evolves in time according to an equation of motion. The equation of motion is a constraint on the allowed behaviour of the field. It expresses the dynamical content of the theory. The solution of that constraint, called the physical field, is the pivotal variable from which we glean all of the physical properties of the system. In addition to dynamical equations, a field theory has a conceptual basis composed of physical assumptions, interpretations and boundary conditions.

The familiar equations of motion, in classical field dynamics, include the Schrödinger equation, Maxwell's equations, Dirac's relativistic equation and several others. In the context of field theory, we call such equations *classical* as long as we are not doing *quantum field theory* (see chapter 15), since the method of solution is directly analogous to that of classical electrodynamics. In spite of this designation, we know that the solutions of Schrödinger's field equation are wavefunctions, i.e. the stuff of quantum mechanics. Whole books have been written about these solutions and their interpretation, but they are not called field theory; they use a different name.

Field theory embraces both quantum mechanics and classical electrodynamics, and goes on to describe the most fundamental picture of matter and energy known to physics. Our aim here is to seek a unified level of description for matter and radiation, by focusing on a field theoretical formulation. This approach allows a uniquely valuable perspective, which forms the basis for the full quantum theory. The equations presented 'classically' in this book have many features in common, although they arise from very different historical threads, but – as we shall see in this chapter – the completeness of the field theoretical description of matter and radiation can only be appreciated by introducing further physical assumptions brought forcefully to bear by Einsteinian relativity. This is discussed in chapter 15.

5.1 Solving the field equations

A solution is a mathematical expression of the balance between the *freedom* expressed by the variables of a theory and the constraints which are implicitly imposed upon them by symmetries and equations of motion.

Each physical model has a limited validity, and each has a context into which one builds its interpretation. Some solutions must be disregarded on the basis of these physical assumptions. Sometimes, additional constraints, such as boundary conditions, are desirable to make contact with the real world. The basic vocabulary of solutions involves some common themes.

5.1.1 Free fields

Free particles or fields do not interact. They experience no disturbances and continue in a fixed state of motion for ever. Free particles are generally described by plane wave fields or simple combinations of plane waves, which may be written as a Fourier transform,

$$\Phi(x) = \int \frac{d^{n+1}k}{(2\pi)^{n+1}} e^{ikx} \Phi(k), \quad (5.1)$$

or, using Schwinger's compact notation for the integration measure, as

$$\Phi(x) = \int (dk) e^{ikx} \Phi(k). \quad (5.2)$$

For this combination to satisfy the field equations, we must add a condition $\chi(k) = 0$, which picks out a hyper-surface (a sub-set) of all of the k_μ which actually satisfy the equations of motion:

$$\Phi(x) = \int (dk) e^{ikx} \Phi_\chi(k) \delta(\chi), \quad (5.3)$$

where $\chi = 0$ is the constraint imposed by the equations of motion on k . Without such a condition, the Fourier transform can represent an arbitrary function. Notice that $\Phi(k)$ and $\Phi_\chi(k)$ have different dimensions by a factor of k due to the delta function. This condition χ is sometimes called the mass shell in particle physics. Elsewhere it is called a dispersion relation. Fields which satisfy this condition (i.e. the equations of motion) are said to be *on shell*, and values of k which do not satisfy this condition are *off shell*. For free fields we have

$$\begin{aligned} \chi_R &= \hbar^2(-\omega^2 + \mathbf{k}^2 c^2) + m^2 c^4 = 0 \\ \chi_{NR} &= \frac{\hbar^2 \mathbf{k}^2}{2m} - \omega = 0, \end{aligned} \quad (5.4)$$

for the relativistic and non-relativistic scalar fields, respectively. The delta-function constraint ensures that the combinations of plane waves obey the

field equations. It has the additional side effect that one component of the wavenumber k_μ is not independent and can be eliminated. It is normal to integrate over the zeroth (energy) component to eliminate the delta function. From Appendix A, eqn. (A.15), we have

$$\Phi(x) = \int (d\mathbf{k}) \left| \frac{\partial \chi}{\partial k_0} \right|^{-1} e^{i(\mathbf{k}\cdot\mathbf{x} - \omega(\mathbf{k})t)} \Phi(\mathbf{k}, \omega(\mathbf{k})). \quad (5.5)$$

Travelling waves carry momentum $k_i > 0$ or $k_i < 0$, while stationary waves carry no momentum, or rather both k_i and $-k_i$ in equal and opposite amounts.

5.1.2 Boundary conditions and causality I

A common strategy for simplifying the analysis of physical systems is to assume that they are infinitely large, or that they are uniform in space and/or time, or that they have been running uniformly in a steady state for ever. Assumptions like this allow one to do away with the complicated behaviour which is associated with the starting up or shutting down of a dynamical process. It also allows one to consider bulk behaviour without dealing with more difficult effects in the vicinity of the edges of a system. Some of the effects of finite size and starting up/shutting down can be dealt with by imposing *boundary conditions* on the behaviour of a system. The term *boundary conditions* is used with a variety of meanings.

- Boundary conditions can be a specification of the absolute value of the field at some specific spacetime points, e.g.

$$\phi(x) \Big|_{x=x_0} = 0. \quad (5.6)$$

This indicates a constraint associated with some inhomogeneity in space-time.

- A corollary to the above is the specification of the value of the field on the walls of a container in a finite system.
- At junctions or interfaces, one is interested in continuity conditions, like those derived in section 4.1.4 and generalizations thereof. Here, one matches the value of the field, perhaps up to a symmetry transformation, across the junction, e.g.

$$\Delta\phi(x_0) = 0, \quad (5.7)$$

meaning that the field does not change discontinuously across a junction. Conditions of this type are sometimes applied to fields, but usually it

is more correct to apply them to conserved quantities such as invariant products of fields, probabilities

$$\Delta(\psi^\dagger\psi) = 0, \quad (5.8)$$

etc. since fields can undergo discontinuous phase changes at boundaries when the topology of spacetime allows or demands it.

- Related to the last case is the issue of spatial topology. Some boundary conditions tell us about the connectivity of a system. For example, a field in a periodic lattice or circle of length L could satisfy

$$\phi(x + L) = U(L)\phi(x). \quad (5.9)$$

In other words, the value of the field is identical, up to a possible phase or symmetry factor $U(L)$, on translating a distance L .

- Another kind of condition which one can impose on a reversible physical system is a direction for causal development. The keywords here are *advanced*, *retarded* and *Feynman boundary conditions* or fluctuations. They have to do with a freedom to change perspective between cause and effect in time-reversible systems. Is the source switched on/off before or after a change in the field? In other words, does the source cause the effect or does it absorb and dampen the effect? This is a matter of viewpoint in reversible systems. The boundary conditions known as Feynman boundary conditions mix these two causal perspectives and provide a physical model for fluctuations of the field or ‘virtual particles’: a short-lived effect which is caused and then absorbed shortly afterwards.

5.1.3 Positive and negative energy solutions

The study of fields in relativistic systems leads to solutions which can be interpreted as having both positive and negative energy. Free relativistic field equations are all transcriptions of the energy relation

$$E = \pm\sqrt{p^2c^2 + m^2c^4}, \quad (5.10)$$

with the operator replacement $p_\mu = -i\hbar\partial_\mu$ and a field on which the operators act. This is most apparent in the case of the Klein–Gordon equation,

$$(-\hbar^2c^2\Box + m^2c^4)\phi(x) = 0. \quad (5.11)$$

Clearly, both signs for the energy are possible from the square-root in eqn. (5.10). The non-relativistic theory does not suffer from the same problem,

since the Schrödinger equation is linear in the energy and the sign is defined to be positive:

$$\frac{\mathbf{p}^2}{2m} = E. \quad (5.12)$$

The field $\phi(x)$ can be expanded as a linear combination of a complete set of plane wavefunctions satisfying the equation of motion. The field can therefore be written

$$\phi(x) = \int (dk) \phi(k) e^{ikx} \delta(\hbar^2 c^2 k^2 + m^2 c^4), \quad (5.13)$$

where $\phi(k)$ are arbitrary coefficients, independent of x . The integral ranges over all energies, but one can separate the positive and negative energy solutions by writing

$$\phi(x) = \phi^{(+)}(x) + \phi^{(-)}(x), \quad (5.14)$$

where

$$\begin{aligned} \phi^{(+)}(x) &= \int (dk) \phi(k) e^{ikx} \theta(k_0) \delta(\hbar^2 c^2 k^2 + m^2 c^4) \\ \phi^{(-)}(x) &= \int (dk) \phi(k) e^{ikx} \theta(-k_0) \delta(\hbar^2 c^2 k^2 + m^2 c^4). \end{aligned} \quad (5.15)$$

The symmetry of the energy relation then implies that

$$\phi^{(+)}(x) = (\phi^{(-)}(x))^*. \quad (5.16)$$

The physical interpretation of negative energy solutions is an important issue, not because negative energy is necessarily unphysical (energy is just a label which embraces a variety of conventions), but rather because there are solutions with arbitrarily large negative energy. A transition from any state to a state with energy $E = -\infty$ would produce an infinite amount of real energy for free. This is contrary to observations and is, presumably, nonsense.

The positive and negative energy solutions to the free relativistic field equations form independently complete sets, with respect to the scalar product,

$$\begin{aligned} (\phi^{(+)}(x), \phi^{(+)}(x)) &= \text{const.} \\ (\phi^{(-)}(x), \phi^{(-)}(x)) &= \text{const.} \\ (\phi^{(+)}(x), \phi^{(-)}(x)) &= 0. \end{aligned} \quad (5.17)$$

In the search for physically meaningful solutions to the free relativistic equations, it might therefore be acceptable to ignore the negative energy solutions on the basis that they are just the mirror image of the positive energy solutions, describing the same physics with a different sign.

This is the case for plane waves, or any solutions which are translationally invariant in time. Such a wave has a time dependence of the form,

$$\phi(t) \sim \exp\left(-i\frac{E}{\hbar}(t - t_0)\right), \quad (5.18)$$

where t_0 is an arbitrary origin for time. If $E < 0$, one can simply recover a positive energy description by moving the origin for time t_0 into the far future, $t_0 \rightarrow \infty$, which essentially switches $t \rightarrow -t$. Since a free particle cannot change its energy by interaction, it will always have a definite energy, either positive or negative. It cannot therefore extract energy from the field by making a transition.

The real problem with negative energies arises in interacting theories. It is not clear how to interpret these solutions from the viewpoint of classical field theory. An extra assumption is needed. This assumption is more clearly justified in the quantum theory of fields (see chapter 15), but is equally valid in the classical theory. The assumption is that there exists a physical state of lowest energy (called the vacuum state) and that states below this energy are interpreted as anti-matter states.

It is sometimes stated that relativistic quantum mechanics (prior to second quantization) is sick, and that quantum field theory is required to make sense of this problem. This is not correct, and would certainly contradict modern thinking about effective field theories.¹ All that is required is a prescription for interpreting the negative energies. The assumptions of quantum field theory, although less well justified, are equally effective and no more arbitrary here. In fact, they are essential since the classical field theory is a well defined limit to the fully quantized field theory.

5.1.4 Sources

The terms *source* and *current* are often used interchangeably in field theory, but they refer to logically distinct entities. Sources (sometimes referred to emphatically as *external sources*) are infinitesimal perturbations to a physical system; currents represent a transfer between one part of a system and another. In an isolated (closed) system, matter and energy can flow from one place to another, and such currents are conserved. There is a close formal similarity between sources and currents, which is no accident. Sources – and their opposites: sinks – can be thought of as infinitesimal currents which are not conserved. They represent the flow of something into or out of a physical system, and thus a perturbation to it. Sources are also the generators of infinitesimal field changes, called virtual processes or fluctuations.

¹ Certain specific Lagrangians lead to unphysical theories, but this is only a reason to reject certain models, not the quantum theory itself.

In mathematics, any quantity on the ‘right hand side’ of a field equation is called a source, ‘forcing term’ or ‘driving term’. A source perturbs or drives the field linearly. For example, consider the Klein–Gordon equation

$$\left(-\square + \frac{m^2 c^2}{\hbar^2}\right)\phi(x) = J. \quad (5.19)$$

One says that $J(x)$ is a source for the field $\phi(x)$. J is sometimes also referred to as a *generalized force*. Sources are included in the action in the form

$$S \rightarrow S + \int (dx) J\phi(x). \quad (5.20)$$

For example, the Klein–Gordon action with a source term becomes

$$S = \int (dx) \left\{ \frac{1}{2} \hbar^2 c^2 (\partial^\mu \phi)(\partial_\mu \phi) + \frac{1}{2} m^2 c^4 \phi^2 - J\phi \right\}. \quad (5.21)$$

When this action is varied, one obtains

$$\frac{\delta S}{\delta \phi} = (-\hbar^2 c^2 \square + m^2 c^4) \phi - J = 0, \quad (5.22)$$

which leads directly to eqn. (5.19). Other source terms include

$$S_{\text{Maxwell}} \rightarrow S_{\text{Maxwell}} + \int (dx) J^\mu A_\mu \quad (5.23)$$

for the electromagnetic field, and

$$S_{\text{complex}} \rightarrow S_{\text{complex}} + \int (dx) \{ J\phi^* + J^*\phi \} \quad (5.24)$$

for a complex scalar field. Most interactions with the field do not have the form of an infinitesimal perturbation. For instance, the interaction with a Schrödinger field, in quantum mechanics, has the form $\psi^* V \psi$, making $J = V \psi$, which is not infinitesimal. However, if one assumes that V is small, or infinitesimal, then this may be expanded around the field ψ for a free theory in such a way that it appears to be a series of infinitesimal impulsive sources; see section 17.5. In this way, the source is the basic model for causal change in the field.

Another definition of the source is by functional differentiation:

$$\frac{\delta S}{\delta \phi_A} = J_A, \quad (5.25)$$

where ϕ is a generic field. This is a generic definition and it follows directly from eqn. (5.20), where one does not treat the source term as part of the action S .

A current represents a flow or transport. To define current, one looks to the only example of current known prior to field theory, namely the electric current. Recall Maxwell's equation

$$\partial_\mu F^{\nu\mu} = \mu_0 J^\nu. \quad (5.26)$$

The quantity J_μ is the $(n + 1)$ dimensional current vector. It is known, from the microscopics of electromagnetism, that this is the electric current: electric currents and electric charges are responsible for the electromagnetic field. However, one may also say that J_μ is a source for the electromagnetic field, because it prevents the left hand side of this equation from being equal to zero. It perturbs the equation of motion. In electromagnetism the current is a source for the field $F_{\mu\nu}$ or A_μ , so it is common to treat source and current as being the same thing. This tendency spills over for other fields too, and one often defines a generic current by eqn. (5.25). Of course, normally one imagines a current as being a vector, whereas the quantity in eqn. (5.25) is a scalar, but this may be used as a definition of 'current'. The notion of conserved currents and their relation to symmetries recurs in chapter 9.

5.1.5 Interactions and measurements

Fields undergo interactions with other fields, and perhaps with themselves (self-interaction). When fields interact with other fields or potentials (either static or dynamical), the state of the field is modified. Classically, the field responds deterministically according to a well defined differential equation (the equation of motion), and interactions apply new constraints. One way to understand weakly interacting systems is to imagine them to be assemblies of weakly-coupled oscillators. In special circumstances, it is possible to construct models with interactions which can be solved exactly. Often, however, approximate methods are required to unravel the behaviour of interacting fields.

In quantum mechanics the act of measurement itself is a kind of temporary interaction, which can lead to a discontinuous change of state. It is not fundamentally different from switching on a potential in field theory. The 'collapse of the wavefunction' thus occurs as a transition resulting from an interaction with a measurement apparatus. This collapse has no detailed description in the theory.

5.2 Green functions and linear response

5.2.1 The inverse problem

Consider an equation of the form

$$\mathcal{D} y(t) = f(t), \quad (5.27)$$

where \mathcal{D} is a differential operator, $y(t)$ is a variable we seek to determine, and $f(t)$ is some forcing term, or ‘source’. We meet this kind of equation repeatedly in field theory, and \mathcal{D} is often an operator of the form $\mathcal{D} = -\square + m^2$.

Normally, one would attempt to solve a differential equation either by integrating it directly, or by ‘substituting in’ a trial solution and looking for consistency. An alternative method is the method of Green functions. The idea can be approached in a number of ways. Let us first take a naive approach.

If \mathcal{D} is an operator, then, if a unique solution to the above equation exists, it must have an inverse. We can therefore write the solution to this equation formally (because the following step has no meaning until we have defined the inverse) by

$$y(t) = (\mathcal{D})^{-1} f(t) = \frac{f(x)}{\mathcal{D}}. \quad (5.28)$$

This is much like the approach used to solve matrix equations in linear algebra. Both the notations in the equation above are to be found in the literature. If the inverse exists, then it must be defined by a relation of the form

$$\frac{\mathcal{D}}{\mathcal{D}} = \mathcal{D} \mathcal{D}^{-1} = I, \quad (5.29)$$

where I is the identity operator.² We do not yet know what these quantities are, but if an inverse exists, then it must be defined in this way. An obvious thing to notice is that our eqn. (5.27) is a differential equation, so the solution involves some kind of integration of the right hand side. Let us now postpone the remainder of this train of thought for a few lines and consider another approach.

The second way in which we can approach this problem is to think of eqn. (5.27) as a ‘linear response’ equation. This means that we think of the right hand side as being a forcing term which perturbs the solution $y(t)$ by kicking it over time into a particular shape. We can decompose the force $f(t)$ into a set of delta-function impulse forces over time,

$$f(t) = \int dt' \delta(t, t') f(t'). \quad (5.30)$$

This equation, although apparently trivial (since it defines the delta function), tells us that we can think of the function $f(t)$ as being a sum of delta functions at different times, weighted by the values of $f(t')$. We can always build up a function by summing up delta functions at different times. In most physical problems we expect the value of $y(t)$ to depend on the past history of all the kicks it has received from the forcing function $f(t)$. This gives us a clue as to how we can define an inverse for the differential operator \mathcal{D} .

² Note that the ordering of the operator and inverse is an issue for differential operators. We require a ‘right-inverse’, but there may be no left inverse satisfying $\mathcal{D}^{-1} \mathcal{D} = I$.

Suppose we introduce a bi-local function $G(t, t')$, such that

$$y(t) = \int dt' G(t, t') f(t'); \quad (5.31)$$

i.e. when we sum up the contributions to the force over time with this weight, it gives us not the force itself at a later time, but the solution. This, in fact, is the way we define the inverse \mathcal{D}^{-1} . It has to be a bi-local function, as we shall see below, and it involves an integration, in spite of the purely formal notation in eqn. (5.29).

Substituting this trial solution into the equation of motion, we have

$$\mathcal{D} \int dt' G(t, t') f(t') = f(t), \quad (5.32)$$

where the operator \mathcal{D} acts on the variable t only, since the dummy variable t' is integrated out from minus to plus infinity. Thus, we may write,

$$\int dt' \overset{t}{\mathcal{D}} G(t, t') f(t') = f(t). \quad (5.33)$$

This equation becomes the defining equation for the delta function (5.30) if and only if

$$\overset{t}{\mathcal{D}} G(t, t') = \delta(t, t'), \quad (5.34)$$

and this equation is precisely of the form of an inverse relation, where the delta function is the identity operator. We have therefore obtained a consistent set of relations which allow us to write a formal solution $y(t)$ in terms of an inverse for the operator $G(t, t')$; we also have an equation which this inverse must satisfy, so the problem has been changed from one of finding the solution $y(t)$ to one of calculating the inverse function. It turns out that this is often an easier problem than trying to integrate eqn. (5.27) directly.

The function $G(t, t')$ goes by several names. It is usually referred to as the *Green('s) function* for the operator \mathcal{D} , but it is also called the *kernel* for \mathcal{D} and, in quantum field theory, the *propagator*.

We can, of course, generalize this function for differential operators which act in an $(n + 1)$ dimensional spacetime. The only difference is that we replace t, t' by x, x' in the above discussion:

$$\begin{aligned} \mathcal{D} y(x) &= f(x) \\ \mathcal{D} G(x, x') &= c\delta(x, x') \\ y(x) &= \int (dx') G(x, x') f(x'). \end{aligned} \quad (5.35)$$

Or, equivalently,

$$\begin{aligned} \mathcal{D}G(x, x') &= \delta(\mathbf{x}, \mathbf{x}')\delta(t, t') \\ y(x) &= \int (dx')G(x, x')f(x'). \end{aligned} \quad (5.36)$$

We are not quite finished with Green functions yet, however: we have skirted around an important issue above, which is described in the next section.

5.2.2 Boundary conditions and causality II

The discussion above is not quite complete: we have written down a function which relates the solution at x to a forcing term at x' via a bi-local function $G(x, x')$. The inverse relation involves an integral over all intermediate times and positions x' , but over what values does this integral run? And over what values of x' was the force defined? Was it switched on suddenly at some time in the past (giving an integral from a fixed time in the past to the present), or has it always existed (giving an integral from minus infinity)? Moreover, why should x' be in the past? We know that physics is usually time-reversible, so why could we not run time backwards and relate a solution in the past to a value of the force in the future, or perhaps a combination of the past and future?

All of these things are possible using different Green functions. We therefore see that the inverse is not unique, and it is not unique because the definition of the inverse involves an integration, and integrals have limits. Physically we are talking about the need to specify initial or boundary conditions on our physical system.

The commonly used Green functions are as follows.

- **Retarded** Green function $G_{\text{r}}(x, x')$. This relates a solution at the present to forces strictly in the past. It is the basis of linear response theory. Due to its origins in electromagnetism, it is often referred to as the *susceptibility* $\chi(x, x') \equiv \chi' + i\chi''$ in other books, with real and imaginary parts as denoted.
- **Advanced** Green function $G_{\text{a}}(x, x')$. This relates a solution at the present to forces strictly in the future.
- **Feynman** Green function $G_{\text{F}}(x, x')$. This relates a solution at the present to forces disposed equally in the past and the future. Its interpretation is rather subtle, since it turns real fields into complex fields as they propagate. The Feynman Green function is a correlation function, and a model for fluctuations in a system. It is sometimes denoted $\Delta(x, x')$, $C(x, x')$ or $S(x, x')$ in other books.

- **Wightman functions.** The positive and negative frequency Wightman functions $G^{(\pm)}(x, x')$ may be thought of as building blocks out of which all the other Green functions may be constructed.

5.2.3 Green functions in Fourier momentum space³

A useful way of calculating quantities is to use an integral transformation, usually the Fourier transformation on the Green functions. The purpose of this step is to turn an operator equation into an ordinary algebraic equation, plus a single integral. This is often referred to as transforming into ‘momentum space’, since the choice of units makes the Fourier transform variables equivalent to momenta.

We shall focus largely on the Green functions for the scalar field, since most of the Green functions for other fields can be obtained from this by differentiation. We are looking to solve an equation of the form

$$(-\square + M^2)G(x, x') = \delta(x, x'), \quad (5.37)$$

where M^2 is some real mass term. We define the Fourier transforms of the Green function by the mutually inverse relations,

$$G(r) = \int (dk) e^{ikr} G(k) \quad (5.38a)$$

$$G(k) = \int (dr) e^{-ikr} G(x, x'), \quad (5.38b)$$

where we have assumed that $G(r) = G(x, x')$ is a translationally invariant function of the coordinates (a function only of the difference $x - x'$), which is reasonable since M^2 is constant with respect to x . We shall also have use for the Fourier representation of the delta function, defined in Appendix A, eqn. (A.10). Notice how the Fourier integral is a general linear combination of plane waves $\exp(ik(x - x'))$, with coefficients $G(k)$. Using this as a solution is just like substituting complex exponentials into differential equations. Substituting these transformed quantities into eqn. (5.37), and comparing the integrands on the left and right hand sides, we obtain

$$(k^2 + M^2)G(k) = 1. \quad (5.39)$$

This is now an algebraic relation which may be immediately inverted and substituted back into eqn. (5.38b) to give

$$G(x, x') = \int (dk) \frac{e^{ik(x-x')}}{k^2 + M^2}. \quad (5.40)$$

³ In this section we set $\hbar = c = 1$ for convenience.

In addition to this ‘particular integral’, one may add to this any linear combination of plane waves which satisfies the mass shell constraint $k^2 + M^2 = 0$. Thus the general solution to the Green function is

$$G_X(x, x') = \int (dk) e^{ik(x-x')} \left[\frac{1}{k^2 + M^2} + X(k, \bar{x}) \delta(k^2 + M^2) \right], \quad (5.41)$$

where $X(k, \bar{x})$ is an arbitrary function of k , and in the unusual case of inhomogeneous systems it can also depend on the average position $\bar{x} = \frac{1}{2}(x + x')$. This arbitrariness in the complementary function is related to the issue of boundary conditions in the previous section and the subsequent discussion in the remainder of this chapter, including the choice of integration path for the Green function. In most cases studied here, $X(k, \bar{x}) = 0$, and we choose a special solution (retarded, advanced, etc.) for the Green function. This term becomes important in satisfying special boundary conditions, and occurs most notably in statistical ‘many-particle’ systems, which vary slowly with \bar{t} away from equilibrium.

We are therefore left with an integral which looks calculable, and this is correct. However, its value is ambiguous for the reason mentioned above: we have not specified any boundary conditions. The ambiguity in boundary conditions takes on the form of a division by zero in the integrand, since

$$k^2 + M^2 = -k_0^2 + \mathbf{k}^2 + M^2 = (\omega_k - k_0)(\omega_k + k_0), \quad (5.42)$$

where $\omega_k = \sqrt{\mathbf{k}^2 + M^2}$. This $G(k)$ has simple poles at

$$k_0 = \pm\omega_k. \quad (5.43)$$

In order to perform the integral, we need to define it unambiguously in the complex plane, by choosing a prescription for going around the poles. It turns out that this procedure, described in many texts, is equivalent to choosing boundary conditions on the Green function.

5.2.4 Limitations of the Green function method

The Green function method nearly always works well in field theory, but it is not without its limitations. The limitations have to do with the order of the differential operator, \mathcal{D} , the number of spacetime dimensions and whether or not the operator contains a mass term. For a massive operator

$$(-\square + M^2)\phi(x) = J(x), \quad (5.44)$$

the general solution is given by

$$\phi(x) = \int (dx) G(x, x') J(x'). \quad (5.45)$$

For a massless field, it is clear that one can always add to this a polynomial of order lower than the order of the differential operator. In the example above, setting $M = 0$ allows us to add

$$\phi(x) = \int (dx) G(x, x') J(x') + \alpha(x - x') + \beta. \quad (5.46)$$

A more serious limitation of the Green function method arises when the order of the differential operator exceeds the number of spacetime dimensions involved in the operator. This leads to non-simple poles in the Green function, which presents problems for the evaluation of the Green function. For example, a second-order operator in one dimension

$$\partial_t^2 G(t, t') = \delta(t, t'). \quad (5.47)$$

If we try to solve this using the Fourier method, we end up with an integral of the form

$$G(t, t') = \int \frac{d\omega}{2\pi} \frac{e^{-i\omega(t-t')}}{-(\omega \pm i\epsilon)^2}. \quad (5.48)$$

This integral has a second-order pole and cannot be used to solve an equation involving ∂_t^2 . For example, the equation for the position of a Newtonian body

$$\partial_t^2 x(t) = F/m, \quad (5.49)$$

cannot be solved in this way since it is not homogeneous in the source F/m . The solution is easily obtained by integration

$$x(t) = \frac{1}{2} \frac{F}{m} t^2 + vt + x_0. \quad (5.50)$$

Since there are terms in this solution which are not proportional to F/m , it is clear that the Green function method cannot provide this full answer. However, the equation can still be solved by the Green function method in two stages.

5.2.5 Green functions and eigenfunction methods

In introductory quantum mechanics texts, the usual approach to solving the system is based on the use of the eigenfunctions of a Hamiltonian operator. This is equivalent to the use of Green functions. The Fourier space expressions given thus far assume that an appropriate expansion can be made in terms of plane wave eigenfunctions:

$$u_k(x) = e^{ikx}. \quad (5.51)$$

Written in this notation, the Green functions have the form

$$G(x, x') = \sum_n G_n u_n(x) u_n^*(x'), \quad (5.52)$$

where the u_n are a complete set of eigenfunctions, or solutions of the field equations, and the G_n are a set of constants in this new expansion. The labels n are sometimes discrete (as in bound state problems) and sometimes continuous, as in the case $n = k$, $G(k)$ and so on. In addition to the above expansion, the question of boundary conditions must be addressed. This can be accomplished by multiplying the coefficients by step functions:

$$G_n(x, x') \propto (\alpha_n \theta(t - t') + \beta_n \theta(t' - t)). \quad (5.53)$$

This is true in many situations, at least when the system concerned is translationally invariant. However, in bound state problems and situations of special symmetry, this expansion leads to an inefficient and sometimes pathological approach.

Consider the relativistic scalar field as an example. The complex scalar field satisfies the equation

$$(-\square + m^2 + V) \phi(x) = J(x). \quad (5.54)$$

Now let φ_n be a complete set of eigenfunctions of the operator in this equation, such that a general wavefunction $\phi(x)$ may be expanded in terms of a complete set of these with coefficients c_n ,

$$\phi(x) = \sum_n c_n \varphi_n(x), \quad (5.55)$$

such that

$$\int d\sigma_x (\varphi_n, \varphi_m) \Big|_{t=t'} = \delta_{nm}. \quad (5.56)$$

The wavefunction $\phi(x)$ and the eigenfunctions $\varphi_n(x)$ are assumed to be one-particle wavefunctions. The discrete indices n, m denote any bound state quantum numbers which the wavefunction might have. The eigenfunctions satisfy

$$(-\square + m^2 + V) \varphi_n(x) = 0. \quad (5.57)$$

The eigenfunctions can also be expressed in terms of their positive and negative frequency parts,

$$\varphi_n(x) = \varphi_n^{(+)}(x) + \varphi_n^{(-)}(x), \quad (5.58)$$

where $\varphi_n^{(+)}(x) = (\varphi_n^{(-)}(x))^*$,

$$\phi_n^{(+)}(x) = \int (dk) e^{ikx} \theta(-k_0) \delta(k^2 + m^2 + V) a_n(k), \quad (5.59)$$

and $a_n(k)$ is a c -number. The Green function for the field (wavefunction) $\phi(x)$ is the inverse of the operator in eqn. (5.54), satisfying,

$$(-\square + m^2 + V) G_{nm}(x, x') = \delta_{nm} \delta(x, x'). \quad (5.60)$$

Using eqn. (5.57) and eqn. (A.21) from Appendix A, we can solve this equation with an object of the form

$$G_{nm} = (\alpha \theta(t - t') + \beta \theta(t' - t)) \sum_{n,m} \varphi_n(x) \varphi_m^*(x'), \quad (5.61)$$

where α and β are to be fixed by the choice of boundary conditions on the Green function.

5.3 Scalar field Green function

The Green function for the scalar field is defined by the relation

$$(-\hbar^2 c^2 \square + m^2 c^4) G(x, x') = \delta(\mathbf{x}, \mathbf{x}') \delta(t, t'). \quad (5.62)$$

It is often convenient to express this in terms of the $(n + 1)$ dimensional delta function

$$\delta(\mathbf{x}, \mathbf{x}') \delta(t, t') = c \delta(\mathbf{x}, \mathbf{x}') \delta(x^0, x'^0) = c \delta(x, x'). \quad (5.63)$$

The right hand side of eqn. (5.62) differs from an $(n + 1)$ dimensional delta function by a factor of c because the action is defined as an integral over $dV_t = (dx)$ rather than dV_x . This convention is chosen because it simplifies the coupling between matter and radiation, and because it makes the Lagrangian density have the dimensions of an energy density. In natural units, $\hbar = c = 1$, this distinction does not arise. The formal expression for the scalar Green function on solving this equation is

$$G(x, x') = c \int (dk) \frac{e^{ik(x-x')}}{p^2 c^2 + m^2 c^4}, \quad (5.64)$$

where $p_\mu = \hbar k_\mu$. Thus, $G(x, x')$ has the dimensions of $\phi^2(x)$. This Green function can be understood in a number of ways. For the remainder of this section, we shall explore its structure in terms of the free-field solutions and the momentum-space constraint surface $p^2 c^2 + m^2 c^4 = 0$, which is referred to in the literature as the 'mass shell'.

5.3.1 The Wightman functions

It is useful to define two quantities, known in quantum field theory as the positive and negative frequency Wightman functions, since all the Green functions can be expressed in terms of these. The Wightman functions are the solutions to the free differential equation,⁴

$$(-\hbar^2 c^2 \square + m^2 c^4)G^{(\pm)}(x, x') = 0. \quad (5.65)$$

For convenience, it is useful to separate the solutions of this equation into those which have positive frequency, $k_0 = |\omega_k|$, and those which have negative frequency, $k_0 = -|\omega_k|$. They may be written by inspection as a general linear combination of plane waves, using a step function, $\theta(\pm k_0)$, to restrict the sign of the frequency, and a delta function to ensure that the integral over all k is restricted only to those values which satisfy the equations of motion,

$$\begin{aligned} G^{(+)}(x, x') &= -2\pi i c \int (dk) e^{ik(x-x')} \theta(-k_0) \delta(p^2 c^2 + m^2 c^4) \\ G^{(-)}(x, x') &= 2\pi i c \int (dk) e^{ik(x-x')} \theta(k_0) \delta(p^2 c^2 + m^2 c^4). \end{aligned} \quad (5.66)$$

Because of unitarity,⁵ these two functions are mutually conjugate (adjoint) in the relativistic theory.

$$G^{(+)}(x, x') = [G^{(-)}(x, x')]^* = -G^{(-)}(x', x). \quad (5.67)$$

In the non-relativistic limit, field theory splits into a separate theory for particles (which have positive energy) and for anti-particles (which have negative energy). Although this relation continues to be true, when comparing the particle theory with the anti-particle theory, it is not true for straightforward Schrödinger theory where the negative frequency Wightman function is zero at zero temperature.

The delta function in the integrands implies that one of the components of the momentum is related to all the others,⁶ thus we may integrate over one of them, k_0 , in order to eliminate this and express it in terms of the others. The equations of motion tell us that $ck_0 = \pm\omega_k$, where

$$\hbar\omega_k = \sqrt{\hbar^2 \mathbf{k}^2 c^2 + m^2 c^4}, \quad (5.68)$$

i.e. there are two solutions, so we may use the identity proven in eqn. (A.15) to write

$$\delta(p^2 c^2 + m^2 c^4) = \frac{1}{2\hbar^2 c^2 |\omega_k|} \left\{ \delta\left(-k_0 + \frac{|\omega_k|}{c}\right) + \delta\left(k_0 + \frac{|\omega_k|}{c}\right) \right\} \quad (5.69)$$

⁴ They are analogous to the complementary function in the theory of linear partial differential equations.

⁵ Unitarity is the property of field theories which implies conservation of energy and probabilities.

⁶ The momentum is said to be 'on shell' since the equation, $k^2 + m^2 = 0$, resembles the equation of a spherical shell in momentum space with radius im .

This relation is valid under the integral sign for k_0 . Noting that the step functions, $\theta(\pm k_0)$, pick out only one or the other delta function on the right hand side, we have

$$\begin{aligned} G^{(+)}(x, x') &= -2\pi i (\hbar^2 c)^{-1} \int \frac{(\mathbf{d}\mathbf{k})}{2\pi} \frac{1}{2\omega_k} e^{i(\mathbf{k}\cdot(\mathbf{x}-\mathbf{x}')-|\omega_k|(t-t'))} \\ G^{(-)}(x, x') &= 2\pi i (\hbar^2 c)^{-1} \int \frac{(\mathbf{d}\mathbf{k})}{2\pi} \frac{1}{2\omega_k} e^{i(\mathbf{k}\cdot(\mathbf{x}-\mathbf{x}')+|\omega_k|(t-t'))} \\ &= 2\pi i (\hbar^2 c)^{-1} \int \frac{(\mathbf{d}\mathbf{k})}{2\pi} \frac{1}{2\omega_k} e^{-i(\mathbf{k}\cdot(\mathbf{x}-\mathbf{x}')-|\omega_k|(t-t'))}. \end{aligned} \quad (5.70)$$

Before leaving this section, we define two further symbols which appear in field theory,

$$\begin{aligned} \tilde{G}(x, x') &= G^{(+)}(x, x') + G^{(-)}(x, x') \\ \overline{G}(x, x') &= G^{(+)}(x, x') - G^{(-)}(x, x'). \end{aligned} \quad (5.71)$$

$\overline{G}(x, x')$ is the sum of all solutions to the free-field equations and, in quantum field theory, becomes the so-called *anti-commutator* function.⁷ Note that this quantity is explicitly the sum of $G^{(+)}(x, x')$ and its complex conjugate $G^{(-)}(x, x')$ and is therefore real in the relativistic theory.⁸

The symmetric and anti-symmetric combinations satisfy the identities

$$\left. \frac{\partial_t^{x'}}{\partial_t} \overline{G}(x, x') \right|_{t=t'} = 0 \quad (5.72)$$

and

$$\left. \frac{\partial_t^{x'}}{\partial_t} \tilde{G}(x, x') \right|_{t=t'} = \delta(\mathbf{x}, \mathbf{x}'). \quad (5.73)$$

The latter turns out to be equivalent to the fundamental commutation relations in the quantum theory of fields. $\tilde{G}(x, x')$ becomes the *commutator* function in the quantum theory of fields.

⁷ This looks wrong from the definitions in terms of Green functions, but recall the signs in the definitions of the Green functions. The tilde denotes the fact that it is a commutator of the quantum fields in the quantum theory.

⁸ This symmetry is broken by the non-relativistic theory as $G^{(-)}(x, x')$ vanishes at the one-particle level.

Finally, we may note that ω_k is always positive, since it is the square-root of a positive, real quantity, so we may drop the modulus signs in future and take this as given.

5.3.2 Boundary conditions and poles in the k_0 plane

When solving differential equations in physics, the choice of boundary conditions normally determines the appropriate mixture of particular integral and complementary functions. The same is true for the Green function approach, but here the familiar procedure is occluded by the formalism of the Green function.

The Wightman functions are the general solutions of the free-field equations: they are the complementary functions, which one may always add to any particular integral. There are two ways to add them to a special solution. One is to use the term X in eqn. (5.41); the other is to deform the complex contour around the poles. This deformation accomplishes precisely the same result as the addition of complementary solutions with complex coefficients. Let us now consider how the deformation of the complex contour leads to the choice of boundary conditions for the field.

The retarded, advanced and Feynman Green functions solve the equations of motion in the presence of a source, with specific boundary conditions as mentioned in section 5.2.2. In this section, we shall impose those boundary conditions and show how this leads to an automatic prescription for dealing with the complex poles in the integrand of eqn. (5.40). The most intuitive way of imposing the boundary conditions is to write the Green functions in terms of the step function:

$$G_r(x, x') = -\theta(\sigma, \sigma')\tilde{G}(x, x') \quad (5.74a)$$

$$G_a(x, x') = \theta(\sigma', \sigma)\tilde{G}(x, x') \quad (5.74b)$$

$$G_F(x, x') = -\theta(\sigma, \sigma')G^{(+)}(x, x') + \theta(\sigma', \sigma)G^{(-)}(x, x'). \quad (5.74c)$$

Note that, since the retarded and advanced Green functions derive from $\tilde{G}(x, x')$, they are real in x, x' space (though this does not mean that their Fourier transforms are real in k space), except in the non-relativistic theory. When we write $\theta(\sigma, \sigma')$ in this way, the σ 's usually refer to two time coordinates $\theta(t, t')$, but in general we may be measuring the development of a system with respect to more general spacelike hyper-surfaces, unconnected with the Cartesian coordinate t or x^0 . For simplicity, we shall refer to t and t' in future. The physical meaning of these functions is as advertised: the retarded function propagates all data from earlier times to later times, the advanced function propagates all data from future times to past times, and the Feynman function takes positive frequency data and propagates them forwards in time, while propagating negative frequency data backwards in time.

To convert these expressions into momentum-space integrals, we make use of the integral representations of the step function,

$$\begin{aligned} \theta(t - t') &= i \lim_{\epsilon \rightarrow 0} \int_{-\infty}^{\infty} \frac{d\alpha}{2\pi} \frac{e^{-i\alpha(t-t')}}{\alpha + i\epsilon} \\ \theta(t' - t) &= -i \lim_{\epsilon \rightarrow 0} \int_{-\infty}^{\infty} \frac{d\alpha}{2\pi} \frac{e^{-i\alpha(t-t')}}{\alpha - i\epsilon}. \end{aligned} \tag{5.75}$$

Writing $\Delta x \equiv x - x'$ for brevity, we can now evaluate these expressions using the momentum-space forms for the Wightman functions in eqn. (5.70).

To evaluate the Green functions in momentum-space, it is useful to employ Cauchy’s residue theorem, which states that the integral around a closed (anti-clockwise) circuit of a function equals 2π times the sum of the residues of the function. Suppose the function $\phi(z)$ has simple poles in the complex plane at z_i , then, assuming that the closed contour is in the anti-clockwise (positive) sense, we have

$$\oint_C \phi(z) dz = 2\pi i \sum_i \left. (z - z_i) \phi(z) \right|_{z=z_i}. \tag{5.76}$$

If the contour C is in the clockwise sense, the sign is reversed.

The complex contour method for evaluating integrals is a useful tool for dealing with Green functions, but one should not confuse the contours with the Green functions themselves. The Green functions we seek are only defined on the real axis, but Cauchy’s formula only works for a closed contour with generally complex pieces. We can evaluate integrals over any contour, in order to use Cauchy’s formula, provided we can extract the value purely along the real axis at the end. The general strategy is to choose a contour so that the contributions along uninteresting parts of the curve are zero.

5.3.3 Retarded Green function

Let us begin with the retarded (causal) Green function, sometimes called the susceptibility χ , and write it as an integral expression in k space. We substitute the integral expressions in eqn. (5.75) into eqn. (5.70) and eqn. (5.74a), giving

$$\begin{aligned} G_r(x, x') &= -\frac{2\pi}{\hbar^2 c} \int \frac{d\alpha}{2\pi} \frac{e^{-i\alpha\Delta t}}{\alpha + i\epsilon} \int \frac{(d\mathbf{k})}{2\pi} \left[\frac{e^{i(\mathbf{k}\Delta\mathbf{x} - \omega_k\Delta t)}}{2\omega_k} - \frac{e^{i(\mathbf{k}\Delta\mathbf{x} + \omega_k\Delta t)}}{2\omega_k} \right] \\ &= -\frac{1}{\hbar^2 c} \int \frac{(d\mathbf{k}) d\alpha}{(2\pi)} \left[\frac{e^{i(\mathbf{k}\Delta\mathbf{x} - (\omega_k + \alpha)\Delta t)}}{2\omega_k(\alpha + i\epsilon)} - \frac{e^{i(\mathbf{k}\Delta\mathbf{x} - (\alpha - \omega_k)\Delta t)}}{2\omega_k(\alpha + i\epsilon)} \right]. \end{aligned} \tag{5.77}$$

We now shift $\alpha \rightarrow \alpha - \omega_k$ in the first term and $\alpha \rightarrow \alpha + \omega_k$ in the second term. This gives

$$G_r(x, x') = - (\hbar^2 c)^{-1} \int \frac{d^n \mathbf{k} d\alpha}{(2\pi)^{n+1}} \frac{e^{i(\mathbf{k}\Delta x - \alpha\Delta t)}}{2\omega_k} \times \left[\frac{1}{(\alpha - \omega_k + i\epsilon)} - \frac{1}{(\alpha + \omega_k + i\epsilon)} \right]. \tag{5.78}$$

Re-labelling $\alpha \rightarrow k_0$ and combining the partial fractions on the right hand side, we are left with,

$$G_r(x, x') = (\hbar^2 c)^{-1} \int (dk) e^{ik\Delta x} \frac{1}{-(k_0 + i\epsilon)^2 + \omega_k^2}, \tag{5.79}$$

or to first order, re-defining $\epsilon \rightarrow \epsilon/2$,

$$G_r(x, x') = c \int (dk) e^{ik\Delta x} \frac{1}{p^2 c^2 + m^2 c^4 - i p_0 \epsilon}. \tag{5.80}$$

This is the significant form we have been looking for. It may be compared with the expression in eqn. (5.40), and we notice that it reduces to eqn. (5.40) in the limit $\epsilon \rightarrow 0$. What is important is that we now have an unambiguous prescription for dealing with the poles: they no longer lie in the real k_0 axis. If we examine the poles of the integrand in eqn. (5.79) we see that they have been shifted below the axis to

$$ck_0 = \pm\omega_k - i\epsilon; \tag{5.81}$$

see figure 5.1. An alternative and completely equivalent contour is shown in figure 5.2. In this approach, we bend the contour rather than shift the poles; the end result is identical.

This $i\epsilon$ prescription tells us how to avoid the poles on the real axis, but it does not tell us how to complete the complex contour. Although the result we are looking for is equal to the value of the integral along the real axis only, Cauchy’s theorem only gives us a prescription for calculating an integral around a closed contour, so we must complete the contour by joining the end of the real axis at $+\infty$ and $-\infty$ with a loop. After that, we extract the value of the portion which lies along the real axis.

The simplest way to evaluate the contribution to such a loop is to make it a semi-circle either in the upper half-plane or in the lower half-plane (see figure 5.2). But which do we choose? In fact, the choice is unimportant as long as we can extract the part of integral along the real axis.

Evaluation around two closed loops We begin by writing the integrals piecewise around the loop in the complex k_0 plane. It is convenient to use $\omega = k_0 c$ as

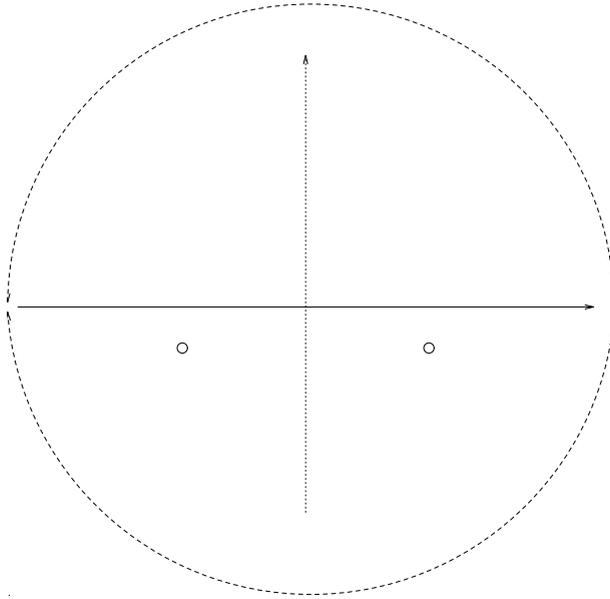


Fig. 5.1. Contour in the complex plane for the retarded Green function with poles shifted using the $i\epsilon$ prescription.

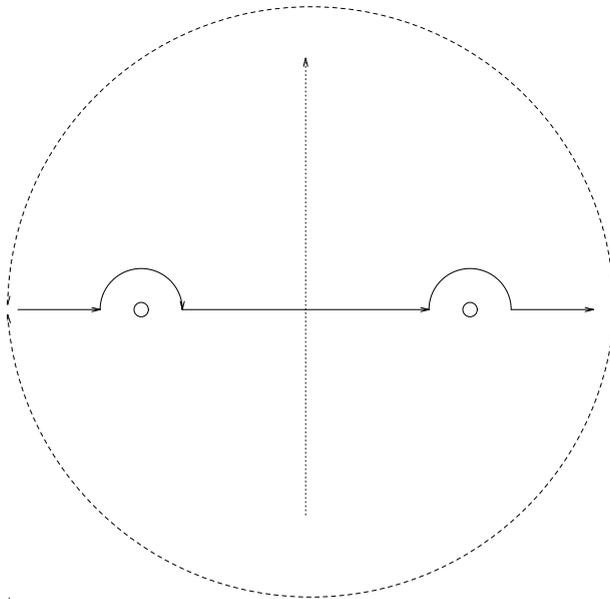


Fig. 5.2. Contour in the complex plane for the retarded Green function.

the integration variable, since this is what appears in the complex exponential. The contour in figure 5.1 has the simplest shape, so we shall use this as our template. We write eqn. (5.79) schematically: the integral over ω is written explicitly, but we absorb all the remaining integrals and the integrand into an object which we shall call $G'_r(k)$ to avoid clutter;

$$\oint d\omega e^{-i\omega(t-t')} G'_r(k) = \int_{-\infty}^{+\infty} d\omega e^{-i\omega(t-t')} G'_r(k) + \int_{SC} d\omega e^{-i\omega(t-t')} G'_r(k), \tag{5.82}$$

where the first term on the right hand side is the piece we wish to find and the second term is the contribution from the semi-circle.

By Cauchy's theorem, the value of the left hand side is equal to $2\pi i$ times the sum of the residues of the integrand which are enclosed by the contour. Since all of the poles lie in the lower half-plane, the left hand side is zero if we complete in the upper half-plane. In the lower half-plane it is

$$\oint d\omega e^{-i\omega(t-t')} G'_r(k) = -2\pi i (\hbar^2 c)^{-1} \int \frac{d^n \mathbf{k}}{(2\pi)^{n+1}} \times \left[\frac{e^{i(\mathbf{k} \cdot \Delta \mathbf{x} + \omega_k \Delta t)}}{-2\omega_k} + \frac{e^{i(\mathbf{k} \cdot \Delta \mathbf{x} - \omega_k \Delta t)}}{2\omega_k} \right] \tag{5.83}$$

Re-labelling $k \rightarrow -k$ in the first term and using

$$e^{ix} - e^{-ix} = 2i \sin(x), \tag{5.84}$$

we have ($\Delta t > 0$)

$$\oint d\omega e^{-i\omega(t-t')} G'_r(k) = \int (\hbar^2 c)^{-1} \frac{d^n \mathbf{k}}{(2\pi)^n} \frac{\cos(\mathbf{k} \cdot \Delta \mathbf{x}) \sin(\omega_k \Delta t)}{\omega_k}. \tag{5.85}$$

This is clearly real.

Semi-circle in the upper half-plane The integral around the semi-circle in the upper half-plane can be parametrized using polar coordinates. We let

$$\omega = r e^{i\theta} = r(\cos \theta + i \sin \theta), \tag{5.86}$$

so that,

$$\begin{aligned} \int_{SC} d\omega e^{-i\omega(t-t')} G'_r(k) &= \int_0^\pi i r e^{i\theta} d\theta e^{-ir(\cos \theta + i \sin \theta)(t-t')} G'_r(r e^{i\theta}) \\ &= \int_0^\pi i r e^{i\theta} d\theta e^{-ir \cos \theta(t-t')} e^{r \sin \theta(t-t')} G'_r(r e^{i\theta}). \end{aligned} \tag{5.87}$$

Note what has happened here. The imaginary component from the semi-circle (the contribution involving $\sin \theta(t - t')$) has created a real exponential. This real exponential causes the integrand to either blow up or decay to zero at $r = \infty$, depending on the sign of the $\sin \theta(t - t')$ term. So we have two cases:

$$\int_{SC} d\omega e^{-i\omega(t-t')} G'_r(k) = 0 \quad (t - t' < 0)$$

$$= ? \quad (t - t' > 0). \tag{5.88}$$

In the first case, in which we do not expect the retarded function to be defined, the integral over the semi-circle vanishes. Since the complete integral around the loop also vanishes here, the real axis contribution that we are looking for (looking at eqn. (5.82)), must also be zero. In the second case, the contribution from the loop is difficult to determine, so the contribution to the real axis part, from eqn. (5.82) is also difficult to determine. In fact, we cannot derive any useful information from this, so for $t - t' > 0$, we cannot determine the value of the integral. In order to evaluate the integral for $t - t' > 0$ we close the contour in the lower half-plane where the semi-circle contribution is again well behaved.

Semi-circle in the lower half-plane The integral around the semi-circle in the lower half-plane can also be parametrized using polar coordinates,

$$\int_{SC} d\omega e^{-i\omega(t-t')} G'_r(k) = - \int_0^{-\pi} i r e^{i\theta} d\theta e^{-ir(\cos \theta + i \sin \theta)(t-t')} G'_r(r e^{i\theta})$$

$$= - \int_0^{-\pi} i r e^{i\theta} d\theta e^{-ir \cos \theta(t-t')} e^{-r |\sin \theta|(t-t')} G'_r(r e^{i\theta}). \tag{5.89}$$

Now the opposite happens:

$$\int_{SC} d\omega e^{-i\omega(t-t')} G'_r(k) = ? \quad (t - t' < 0)$$

$$= 0 \quad (t - t' > 0). \tag{5.90}$$

This time the situation is reversed. The value of the integral tells us nothing for $t - t' < 0$. In the second case, however, the contribution to the loop goes to zero, making the integral along the real axis equal to the loop integral result in eqn. (5.85).

Piece-wise definition Because of the infinite pieces, we must close the contour for the retarded Green function separately for $t - t' > 0$ (lower half-plane, non-zero result) and $t - t' < 0$ (upper half-plane, zero result). This is not a serious problem for evaluating single Green functions, but the correct choice of contour becomes more subtle when calculating products of Green functions

using the momentum-space forms. We have nonetheless established that these momentum-space prescriptions lead to a Green function which propagates from the past into the future:

$$G_r(x, x') = (\hbar^2 c)^{-1} \int \frac{d^n \mathbf{k}}{(2\pi)^n} \frac{\cos(\mathbf{k} \cdot \Delta \mathbf{x}) \sin(\omega_k \Delta t)}{\omega_k} \quad (t - t' > 0)$$

$$= 0 \quad (t - t' < 0). \quad (5.91)$$

5.3.4 Advanced Green function

The treatment of this function is identical in structure to that for the retarded propagator. The only difference is that the poles lie in the opposite half-plane, and thus the results are reversed:

$$G_a(x, x') = - (\hbar^2 c)^{-1} \int (dk) e^{ik\Delta x} \frac{1}{-(k_0 - i\epsilon)^2 + \omega_k^2}. \quad (5.92)$$

We see that the poles are shifted above the axis and that the complex contour may now be completed in the opposite manner to the retarded Green function. The result is

$$G_a(x, x') = - (\hbar^2 c)^{-1} \int \frac{d^n \mathbf{k}}{(2\pi)^n} \frac{\sin(\mathbf{k} \cdot \Delta \mathbf{x} - \omega_k \Delta t)}{\omega_k} \quad (t - t' < 0)$$

$$= 0 \quad (t - t' > 0). \quad (5.93)$$

5.3.5 Feynman Green function

$$G_F(x, x') = - \frac{2\pi}{\hbar^2 c} \int \frac{d\alpha}{2\pi} \frac{d\mathbf{k}}{(2\pi)} \left[\frac{e^{i(\mathbf{k}\Delta\mathbf{x} - (\omega_k + \alpha)\Delta t)}}{(\alpha + i\epsilon)2\omega_k} - \frac{e^{i(\mathbf{k}\Delta\mathbf{x} - (\alpha - \omega_k)\Delta t)}}{(\alpha - i\epsilon)2\omega_k} \right]. \quad (5.94)$$

Shifting $\alpha \rightarrow \alpha - \omega_k$ in the first fraction and $\alpha \rightarrow \alpha + \omega_k$ in the second fraction, and re-labelling $\alpha \rightarrow k_0$ we obtain,

$$G_F(x, x') = (\hbar^2 c)^{-1} \int (dk) \frac{e^{ik\Delta x}}{2\omega_k} \left[\frac{1}{(k_0 + \omega_k - i\epsilon)} - \frac{1}{(k_0 - \omega_k + i\epsilon)} \right]. \quad (5.95)$$

It is normal to re-write this in the following way. Remember that we are interested in the limit $\epsilon \rightarrow 0$. Combining the partial fractions above, we get

$$G_F(x, x') = (\hbar^2 c)^{-1} \int (dk) e^{ik\Delta x} \left[\frac{-1}{(k_0 + \omega - i\epsilon)(k_0 - \omega + i\epsilon)} + O(\epsilon) \right]. \quad (5.96)$$

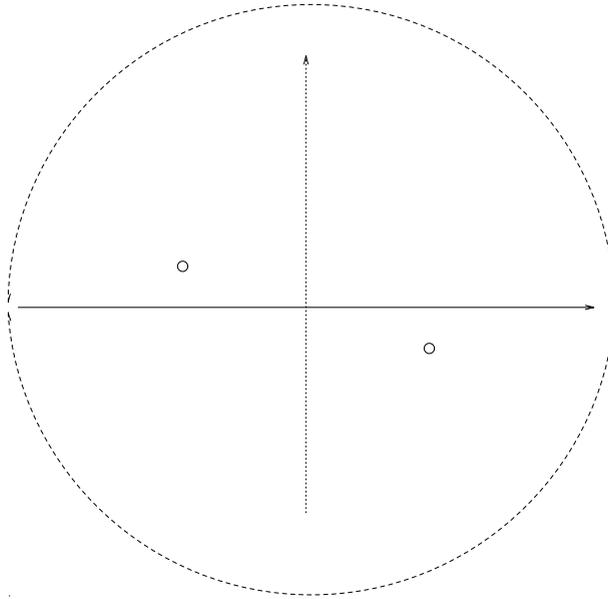


Fig. 5.3. Contour in the complex plane for the Feynman Green function. This shows how the $i\epsilon$ prescription moves the poles effectively from the real axis.

From this expression, we see that the poles have been shifted from the real axis to

$$\begin{aligned} ck_0 &= \omega_k - i\epsilon \\ ck_0 &= -\omega_k + i\epsilon, \end{aligned} \quad (5.97)$$

i.e. the negative root is shifted above the axis and the positive root below the axis in the k_0 plane (see figure 5.4). An equivalent contour is shown in figure 5.3. Although it does not improve one's understanding in any way, it is normal in the literature to write the Feynman Green function in the following way. Re-writing the denominator, we have

$$(ck_0 + \omega - i\epsilon)(ck_0 - \omega + i\epsilon) = c^2k_0^2 - \omega_k^2 + 2i\epsilon\omega_k + \epsilon^2. \quad (5.98)$$

Now, since ϵ is infinitesimal and $\omega_k > 0$, we may drop ϵ^2 , and write $2i\epsilon\omega_k = i\epsilon'$. This allows us to write

$$G_F(x, x') = c \int (dk) \frac{e^{ik\Delta x}}{p^2c^2 + m^2c^4 - i\epsilon'}. \quad (5.99)$$

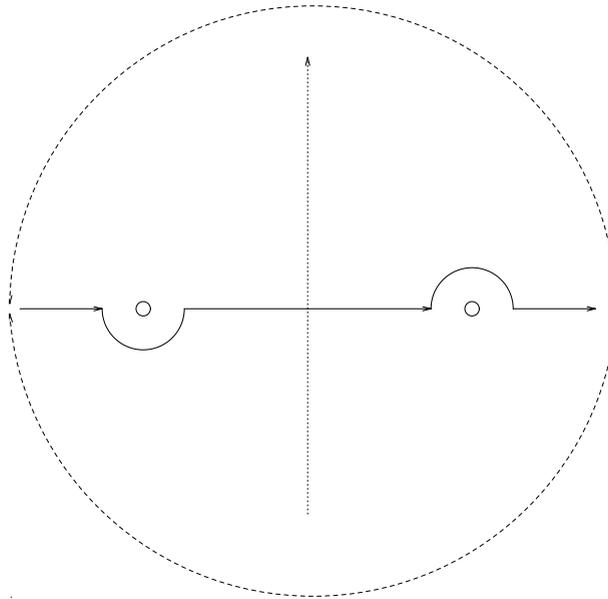


Fig. 5.4. Contour in the complex plane for the Feynman Green function. Here we bend the contour rather than moving the poles. The result is identical.

5.3.6 Comment on complex contours

The procedure described by Green functions is a formalism for extracting solutions to the inverse-operator problem. It has a direct analogy in the theory of matrices or linear algebra. There the issue concerns the invertibility of matrices and the determinant of the matrix operator. Suppose we have a matrix equation

$$M \cdot \mathbf{x} = \mathbf{J}, \quad (5.100)$$

with a matrix M given by

$$M = \begin{pmatrix} a & b \\ c & d \end{pmatrix}. \quad (5.101)$$

If this matrix has an inverse, which is true if the determinant $ad - bc$ does not vanish,

$$M^{-1} = \frac{1}{ad - bc} \begin{pmatrix} d & -b \\ -c & a \end{pmatrix}, \quad (5.102)$$

then eqn. (5.100) has a unique solution. We would not expect this case to correspond to the solution of a differential equation such as the one we are considering, since we know that the general solution to second-order differential equations usually involves a linear super-position of many solutions.

If the determinant of M does vanish, then it means that there is an infinite number of solutions, which corresponds to a sub-space of x (a hyper-surface which is determined by a constraint linking the coordinates). In this case, the inverse defined above in eqn. (5.102) has a pole. For example, suppose we take M to be the matrix

$$M = \begin{pmatrix} 1 & 2 & 1 \\ 1 & 1 & 0 \\ 4 & 8 & 4 \end{pmatrix}, \quad (5.103)$$

and

$$J = \begin{pmatrix} 4 \\ 2 \\ 16 \end{pmatrix}. \quad (5.104)$$

This matrix clearly has no inverse, since the third row is a multiple of the first. The determinant vanishes, but in this trivial case we can solve the equations directly. Since there are only two independent equations and three unknowns, it is not possible to find a unique solution. Instead, we eliminate all but one of the variables, leaving

$$x_2 + x_3 = 2. \quad (5.105)$$

This is the equation of a straight line, or a sub-space of the full three-dimensional solution space. We regard this as an incomplete constraint on the solution space rather than a complete solution.

This is analogous to the situation we have with the Green functions. The poles indicate that the solution to the differential equation which we are trying to solve is not unique. In fact, there is an infinite number of plane wave solutions which lie on the hyper-surface $k^2 + m^2 = 0$, called the mass shell.

5.4 Scalar Green functions in real space

Although the momentum-space representations of the Green functions are useful for calculations, we are usually interested in their forms in real space. For general fields with a mass, these can be quite complicated, but in the massless limit the momentum-space integrals can be straightforwardly evaluated.

Again, since the other relativistic Green functions can be expressed in terms of that for the scalar field, we shall focus mainly on this simple case.

5.4.1 The retarded Green function for $n = 3$ as $m \rightarrow 0$

From Cauchy’s residue theorem in eqn. (5.76), we have

$$G_r(x, x') = -2\pi i (\hbar^2 c)^{-1} \int \frac{d^3 \mathbf{k}}{(2\pi)^4} \left[\frac{e^{i(\mathbf{k} \cdot \Delta \mathbf{x} - \omega_k \Delta t)}}{2\omega_k} - \frac{e^{i(\mathbf{k} \cdot \Delta \mathbf{x} + \omega_k \Delta t)}}{2\omega_k} \right]. \tag{5.106}$$

For general $m \neq 0$, this integral defines Bessel functions. For $m = 0$, however, the integral is straightforward and can be evaluated by going to three-dimensional polar coordinates in momentum space:

$$\begin{aligned} \omega_k &= |r|c \\ \int d^3 \mathbf{k} &= \int_0^\infty r^2 dr \int_0^\pi \sin \theta d\theta \int_0^{2\pi} d\phi \\ \mathbf{k} \cdot \mathbf{x} &= |r| \Delta X \cos \theta, \end{aligned} \tag{5.107}$$

where $\Delta X = |\Delta \mathbf{x}|$, so that

$$\begin{aligned} G_r(x, x') &= \frac{-i}{16\pi^3} (\hbar^2 c)^{-1} \int_0^\infty 2\pi r^2 dr \\ &\times \int_0^\pi \sin \theta d\theta \frac{e^{ir\Delta x \cos \theta}}{r} [e^{-irc\Delta t} - e^{irc\Delta t}]. \end{aligned} \tag{5.108}$$

The integral over $d\theta$ may now be performed, giving

$$\begin{aligned} G_r(x, x') &= \frac{-1}{8\pi^2 \Delta X} (\hbar^2 c)^{-1} \int_0^\infty dr \left\{ e^{-ir(\Delta X + c\Delta t)} \right. \\ &\quad \left. - e^{ir(\Delta t - c\Delta X)} - e^{ir(\Delta X - c\Delta t)} + e^{ir(\Delta X + c\Delta t)} \right\}. \end{aligned} \tag{5.109}$$

Note that both Δt and Δx are positive by assumption. From the definition of the delta function, we have

$$\begin{aligned} 2\pi \delta(x) &= \int_{-\infty}^{+\infty} dk e^{ikx} \\ &= \int_0^\infty [e^{ikx} + e^{-ikx}]. \end{aligned} \tag{5.110}$$

Using this result, we see that the first and last terms in eqn. (5.109) vanish, since Δx can never be equal to $-\Delta t$ as both Δx and Δt are positive. This leaves us with

$$\begin{aligned} G_r(x, x') &= \frac{1}{4\hbar^2 c\pi \Delta X} \delta(ct - \Delta X) \\ &= \frac{1}{4\pi \hbar^2 c |\mathbf{x} - \mathbf{x}'|} \delta(c(t - t') - |\mathbf{x} - \mathbf{x}'|). \end{aligned} \tag{5.111}$$

5.4.2 The $G^{(\pm)}$ and G_F for $n = 3$ as $m \rightarrow 0$

From eqn. (5.74c) we can see that the Feynman propagator is manifestly equal to $-G^{(+)}$ for $t > t'$ and is equal to $G^{(-)}$ for $t' < t$. The calculation of all three quantities can therefore be taken together. We could, in fact, write this down from the definitions, but it is useful to use the residue theorem on eqn. (5.95) to show the consistency of the procedure with the definitions we have already given. In fact, we shall see that the Wightman functions *are* just the residues, up to a sign which depends on the orientation of the closed contour.

For $t - t' > 0$, we complete the contour in the lower half-plane, creating an anti-clockwise contour. The residue theorem then tells us that

$$\oint dk_0 G'_F(k_0) = (\hbar^2 c)^{-1} \int \frac{d(\mathbf{k})}{(2\pi)} \frac{1}{2\omega_k} e^{ik\Delta x} \times -2\pi i \{-1\} \Big|_{k_0=\omega_k} \quad (5.112)$$

Comparing this equation with eqns. (5.66), we see that this is precisely equal to $-G^{(+)}(x, x')$. In the massless limit with $n = 3$, we may therefore write

$$\begin{aligned} G^{(+)} &= -i (\hbar^2 c)^{-1} \frac{d^3\mathbf{k}}{(2\pi)^4} \frac{e^{ik\Delta x}}{2|\mathbf{k}|c^2} \\ &= \frac{-1}{8\pi^2 \hbar^2 c |\mathbf{x}' - \mathbf{x}|} \int_0^\infty dr \{e^{-ir(\Delta X + c\Delta t)} - e^{ir(\Delta X - c\Delta t)}\}. \end{aligned} \quad (5.113)$$

Similarly, for $t - t' < 0$, we complete the contour in the upper half-plane, creating a clockwise contour. This gives

$$\oint dk_0 G'_F(k_0) = (\hbar^2 c)^{-1} \int \frac{d(\mathbf{k})}{(2\pi)} \frac{1}{2\omega_k} e^{i(\mathbf{k}\cdot\Delta\mathbf{x} + \omega_k\Delta t)} \times 2\pi i \{+1\} \Big|_{k_0=\omega_k} \quad (5.114)$$

Comparing this equation with eqn. (5.66), we see that this is precisely equal to $G^{(-)}(x, x')$, and

$$G^{(-)} = \frac{1}{8\pi^2 \hbar^2 c |\mathbf{x}' - \mathbf{x}|} \int_0^\infty dr \{e^{-ir(\Delta X - c\Delta t)} - e^{ir(\Delta X + c\Delta t)}\}. \quad (5.115)$$

It may be checked that these expressions satisfy eqn. (5.67). Finally, we may piece together the Feynman Green function from $G^{(\pm)}$. Given that the Δt are assumed positive, we have

$$\begin{aligned} G_F(x, x') &= \frac{1}{8\pi^2 \hbar^2 c |\mathbf{x} - \mathbf{x}'|} \int_0^\infty dr \{e^{-ir(\Delta X)} - e^{ir(\Delta X)} e^{-irc\Delta t}\} \\ &= \frac{-i}{4\pi^2 \hbar^2 c |\mathbf{x} - \mathbf{x}'|} \int_0^\infty dr \sin(r|\mathbf{x}' - \mathbf{x}|) e^{-irc|t-t'|}. \end{aligned} \quad (5.116)$$

We may note that the difference between the retarded and Feynman Green functions is

$$\begin{aligned} G_F(x, x') - G_r(x, x') &= \lim_{\alpha \rightarrow 0} 2 \int_0^\infty dr e^{ir(c\Delta t - \Delta X + i\alpha)} - e^{ir(c\Delta t + \Delta X + i\alpha)} \\ &= \frac{i}{|\mathbf{x} - \mathbf{x}'| - c|t - t'|} - \frac{i}{|\mathbf{x} + \mathbf{x}'| - c|t - t'|}, \end{aligned} \quad (5.117)$$

where α is introduced to define the infinite limit of the complex exponential. This difference is a purely imaginary number, which diverges on the light cone.

5.4.3 Frequency-dependent form of G_F and G_r in $n = 3$

In atomic physics and optics, one usually deals in implicitly translational invariant systems, in the rest frames of an atom, where the frequency ω and time are the only variables entering physical models. To use standard field theoretical methods in these cases, it is useful to have the Green functions in such a form, by integrating over spatial wavenumbers leaving only the Fourier transform over time. These are obtained trivially by re-writing the non-zero contributions to eqns. (5.109) and (5.116) with $r \rightarrow \omega/c$:

$$\begin{aligned} G_F(x, x') &= \frac{-i}{4\pi^2 \hbar^2 c^2 |\mathbf{x} - \mathbf{x}'|} \int_0^\infty d\omega \sin\left(\frac{\omega}{c} |\mathbf{x} - \mathbf{x}'|\right) e^{-i\omega|t-t'|} \\ G_r(x, x') &= \frac{1}{4\pi^2 \hbar^2 c^2 |\mathbf{x} - \mathbf{x}'|} \int_0^\infty d\omega \cos\left(\frac{\omega}{c} |\mathbf{x} - \mathbf{x}'| - \omega|t - t'|\right). \end{aligned} \quad (5.118)$$

5.4.4 Euclidean Green function in $2 + 0$ dimensions

In the special case of a space-only Green function (the inverse of the Laplacian operator), there is no ambiguity in the boundary conditions, since the Green function is time-independent and there are no poles in the integrand. Let us define the inverse Laplacian by

$$(-\nabla^2 + m^2)g(x, x') = \delta(x, x'). \quad (5.119)$$

To evaluate this function, we work in Fourier space and write

$$g(x, x') = \int \frac{d^2k}{(2\pi)^2} \frac{e^{ik(x-x')}}{k^2 + m^2}, \quad (5.120)$$

where $k^2 = k_1^2 + k_2^2$. Expressing this in polar coordinates, we have

$$g(x, x') = \int_0^{2\pi} \int_0^\infty \frac{r dr d\theta}{(2\pi)^2} \frac{e^{ir|x-x'|\cos\theta}}{r^2 + m^2}. \quad (5.121)$$

Massless case In the massless limit, this integral can be evaluated straightforwardly using a trick which is frequently useful in the evaluation of Fourier integrals. The trick is only valid strictly when $x \neq x'$, but we shall leave it as an exercise to show what happens in that case. The integral is then evaluated by setting m to zero in eqn. (5.121) and cancelling a factor of r from the integration measure. To evaluate the expression, we differentiate under the integral sign with respect to the quantity $|x - x'|$:

$$\frac{d}{d|x - x'|} g(x - x') = \int_0^{2\pi} \int_0^\infty \frac{i \cos \theta}{(2\pi)^2} e^{ir|x-x'|\cos\theta} dr d\theta. \quad (5.122)$$

Notice that this step cancels a factor of r in the denominator, which means that the integral over r is now much simpler. Formally, we have

$$\frac{d}{d|x - x'|} g(x - x') = \int_0^{2\pi} \frac{d\theta}{(2\pi)^2} e^{ir|x-x'|\cos\theta} \Big|_0^\infty. \quad (5.123)$$

There is still a subtlety remaining, however: since we are integrating a complex, multi-valued function, the limit at infinity has an ambiguous limit. The limit can be defined uniquely (analytically continued) by adding an infinitesimal positive imaginary part to r , so that $r \rightarrow r(i + \epsilon)$ and letting $\epsilon \rightarrow 0$ afterwards. This makes the infinite limit converge to zero, leaving only a contribution from the lower limit:

$$\begin{aligned} \frac{d}{d|x - x'|} g(x - x') &= \lim_{\epsilon \rightarrow 0} \int_0^{2\pi} \frac{d\theta}{(2\pi)^2} \frac{1}{1 - i\epsilon} e^{(ir - \epsilon r)|x-x'|\cos\theta} \Big|_0^\infty \\ &= - \int_0^{2\pi} \frac{d\theta}{(2\pi)^2} \frac{1}{|x - x'|}. \end{aligned} \quad (5.124)$$

To complete the evaluation, we evaluate the two remaining integrals trivially, first the anti-derivative with respect to $|x - x'|$, which gives rise to a logarithm, and finally the integral over θ , giving:

$$g(x, x') = -\frac{1}{2\pi} \ln |x - x'|, \quad (5.125)$$

where it is understood that $x \neq x'$.

5.4.5 Massive case

In the massive case, we can write down the result in terms of Bessel functions J_ν , K_ν , by noting the following integral identities [63]:

$$J_\nu(z) = \frac{(z/2)^\nu}{\Gamma(\nu + \frac{1}{2})\Gamma(\frac{1}{2})} \int_0^\pi e^{\pm iz \cos \theta} \sin^{2\nu} \theta d\theta \quad (5.126)$$

$$K_{\nu-\mu}(ab) = \frac{2^\mu \Gamma(\mu + 1)}{a^{\nu-\mu} b^\mu} \int_0^\infty \frac{J_\nu(bx) x^{\nu+1}}{(x^2 + a^2)} dx. \quad (5.127)$$

From the first of these, we can choose $\nu = 0$ and use the symmetry of the cosine function to write

$$J_0(z) = \frac{1}{2\pi} \int_0^{2\pi} e^{iz \cos \theta} d\theta. \tag{5.128}$$

Eqn. (5.121) may now be expressed in the form

$$g(x, x') = \int_0^\infty \frac{r dr}{2\pi} \frac{J_0(r|x - x'|)}{r^2 + m^2}, \tag{5.129}$$

and hence

$$g(x, x') = \frac{1}{2\pi} K_0(m|x - x'|). \tag{5.130}$$

The massless limit is singular, but with care can be inferred from the small argument expansion

$$K_0(m(x - x')) = \lim_{m \rightarrow 0} -\ln \left(\frac{m(x - x')}{2} \right) \sum_{k=0}^\infty \frac{\left(\frac{m(x-x')}{2} \right)^{2k}}{(k!)^2}. \tag{5.131}$$

5.5 Schrödinger Green function

Being linear in the time derivative, the solutions of the Schrödinger equation have positive definite energy. The Fourier transform may therefore be written as,

$$\psi(x) = \int_0^\infty \frac{d\tilde{\omega}}{2\pi} \int_{-\infty}^{+\infty} (d\mathbf{k}) e^{i(\mathbf{k} \cdot \Delta\mathbf{x} - \tilde{\omega}\Delta t)} \psi(\mathbf{k}, \tilde{\omega}) \theta(\tilde{\omega}) \delta \left(\frac{\hbar^2 \mathbf{k}^2}{2m} - \hbar\tilde{\omega} \right). \tag{5.132}$$

This singles out the Schrödinger field amongst the other relativistic fields which have solutions of both signs. Correspondingly, the Schrödinger field has only a positive energy Wightman function, the negative energy function vanishes from the particle theory.⁹ The positive frequency Wightman function is

$$G_{\text{NR}}^{(+)}(x, x') = -2\pi i \int_0^\infty \frac{d\tilde{\omega}}{2\pi} \int_{-\infty}^{+\infty} (d\mathbf{k}) e^{i(\mathbf{k} \cdot \Delta\mathbf{x} - \tilde{\omega}\Delta t)} \theta(\tilde{\omega}) \delta \left(\frac{\hbar^2 \mathbf{k}^2}{2m} - \hbar\tilde{\omega} \right). \tag{5.133}$$

The negative frequency Wightman function vanishes now,

$$G_{\text{NR}}^{(-)}(x, x') = 0, \tag{5.134}$$

⁹This does not remain true at finite temperature or in interacting field theory, but there remains a fundamental asymmetry between positive and negative energy Green functions in the non-relativistic theory.

since there is no pole in the negative $\tilde{\omega}$ plane to enclose. Moreover, this means that there is no Feynman Green function in the non-relativistic theory, only a retarded one. In the non-relativistic limit, both the Feynman Green function and the retarded Green function for relativistic particles reduce to the same result, which has poles only in the lower half complex $\tilde{\omega}$ plane. This non-relativistic Green function satisfies the equation

$$\left(-\frac{\hbar^2 \nabla^2}{2m} - i\hbar \partial_t\right) G_{\text{NR}}(x, x') = \delta(\mathbf{x}, \mathbf{x}') \delta(t, t'). \quad (5.135)$$

This Green function can be evaluated from the expression corresponding to those in eqns. (5.74):

$$G_{\text{NR}}(x, x') = -\theta(t - t') G_{\text{NR}}^{(+)}(x, x'). \quad (5.136)$$

Using eqn. (5.75) in eqn. (5.133), we have

$$G_{\text{NR}}(x, x') = -\int_{-\infty}^{+\infty} d\alpha \int_0^{\infty} \frac{d\tilde{\omega}}{2\pi} \int_{-\infty}^{+\infty} (d\mathbf{k}) \times \frac{e^{i(\mathbf{k} \cdot \Delta \mathbf{x} - (\tilde{\omega} + \alpha)\Delta t)}}{(\alpha + i\epsilon)} \delta\left(\frac{\hbar^2 \mathbf{k}^2}{2m} - \hbar \tilde{\omega}\right). \quad (5.137)$$

The integral over α can be shifted, $\alpha \rightarrow \alpha - \tilde{\omega}$, without consequences for the limits or the measure, giving

$$G_{\text{NR}}(x, x') = -\int_{-\infty}^{+\infty} d\alpha \int_0^{\infty} \frac{d\tilde{\omega}}{2\pi} \int_{-\infty}^{+\infty} (d\mathbf{k}) \times \frac{e^{i(\mathbf{k} \cdot \Delta \mathbf{x} - \alpha \Delta t)}}{(\alpha - \tilde{\omega}) + i\epsilon} \delta\left(\frac{\hbar^2 \mathbf{k}^2}{2m} - \hbar \tilde{\omega}\right). \quad (5.138)$$

We may now integrate over $\tilde{\omega}$ to invoke the delta function. Noting that the argument of the delta function is defined only for positive $\tilde{\omega}$, and that the integral is also over this range, we have simply

$$G_{\text{NR}}(x, x') = -\int_{-\infty}^{+\infty} d\alpha \int_{-\infty}^{+\infty} (d\mathbf{k}) \frac{e^{i(\mathbf{k} \cdot \Delta \mathbf{x} - \alpha \Delta t)}}{\left(\hbar \alpha - \frac{\hbar^2 \mathbf{k}^2}{2m}\right) + i\epsilon}, \quad (5.139)$$

or, re-labelling $\alpha \rightarrow \tilde{\omega}$,

$$G_{\text{NR}}(x, x') = \int_{-\infty}^{+\infty} d\tilde{\omega} \int_{-\infty}^{+\infty} (d\mathbf{k}) \frac{e^{i(\mathbf{k} \cdot \Delta \mathbf{x} - \tilde{\omega} \Delta t)}}{\left(\frac{\hbar^2 \mathbf{k}^2}{2m} - \hbar \tilde{\omega}\right) - i\epsilon}. \quad (5.140)$$

In spite of appearances, the parameter $\tilde{\omega}$ is not really the energy of the system, since it runs from minus infinity to plus infinity. It should properly be regarded

only as a variable of integration. It is clear from this expression that the Schrödinger field has a single pole in the lower half complex plane. It therefore satisfies purely retarded boundary conditions. We shall see in section 13.2.2 how the relativistic Feynman Green function reduces to a purely retarded one in the non-relativistic limit.

5.6 Dirac Green functions

The Dirac Green function satisfies an equation which is first order in the derivatives, but which is matrix-valued. The equation of motion for the Dirac field,

$$(-i\gamma^\mu \partial_\mu + m)\psi = J, \quad (5.141)$$

tells us that a formal solution may be written as

$$\psi = \int dV_{x'} S(x, x') J(x'), \quad (5.142)$$

where the spinor Green function is defined by

$$(-i\hbar c \gamma^\mu \partial_\mu + mc^2)S(x, x') = \delta(x, x'). \quad (5.143)$$

Although this looks rather different to the scalar field case, $S(x, x')$ can be obtained from the expression for the scalar propagator by noting that

$$\begin{aligned} & (-i\hbar c \gamma^\mu \partial_\mu + mc^2)(i\hbar c \gamma^\mu \partial_\mu + mc^2) \\ &= -\hbar^2 c^2 \square + m^2 c^4 + \frac{1}{2}[\gamma^\mu, \gamma^\nu] \partial_\mu \partial_\nu, \end{aligned} \quad (5.144)$$

and the latter term vanishes when operating on non-singular objects. It follows for the free field that

$$(i\hbar c \gamma^\mu \partial_\mu + mc^2)G^{(\pm)}(x, x') = S^{(\pm)}(x, x') \quad (5.145)$$

$$(i\hbar c \gamma^\mu \partial_\mu + mc^2)G_F(x, x') = S_F(x, x') \quad (5.146)$$

$$(-i\hbar c \gamma^\mu \partial_\mu + mc^2)S^{(\pm)}(x, x') = 0 \quad (5.147)$$

$$(-i\hbar c \gamma^\mu \partial_\mu + mc^2)S_F(x, x') = \delta(x, x'). \quad (5.148)$$

5.7 Photon Green functions

The Green function for the Maxwell field satisfies the $(n+1)$ dimensional vector equation

$$[-\square \delta_\mu^\nu + \partial_\mu \partial^\nu] A^\mu(x) = \mu_0 J^\nu. \quad (5.149)$$

As usual, we look for the inverse of the operator,¹⁰ which satisfies

$$[-\square \delta_\mu^\nu + \partial_\mu \partial^\nu] D_\nu^\rho(x, x') = \mu_0 c \delta_\mu^\rho \delta(x, x'). \tag{5.150}$$

Formally, it can be written as a Fourier transform:

$$D_{\mu\nu}(x, x') = \mu_0 c \int (dk) e^{ik(x-x')} \left[\frac{g_{\mu\nu}}{k^2} - \frac{k^\mu k^\nu}{k^4} \right]. \tag{5.151}$$

In this case, however, there is a problem. In inverting the operator, we are looking for a constraint which imposes the equations of motion. For scalar particles, this is done by going to momentum space and constructing the Green function, which embodies the equations of motion in the dispersion relation $k^2 + m^2 = 0$ (see eqn. (5.40)). In this case, that approach fails.

The difficulty here is the gauge symmetry. Suppose we consider the determinant of the operator in eqn. (5.149). A straightforward computation shows that this determinant vanishes:

$$\begin{vmatrix} -\square + \partial_0 \partial^0 & \partial_0 \partial^i \\ \partial_i \partial^0 & -\square + \partial_i \partial^i \end{vmatrix} = 0. \tag{5.152}$$

In linear algebra, this would be a signal that the matrix was not invertible, the matrix equivalent of dividing by zero. It also presents a problem here. The problem is not that the operator is not invertible (none of the Green function equations are invertible when the constraints they impose are fulfilled, since they correspond precisely to a division by zero), but rather that it implies no constraint at all. In the case of a scalar field, we have the operator constraint, or its momentum-space form:

$$\begin{aligned} -\hbar^2 c^2 \square + m^2 c^4 &= 0 \\ p^2 c^2 + m^2 c^4 &= 0. \end{aligned} \tag{5.153}$$

In the vector case, one has

$$\det [-\square \delta_\mu^\nu + \partial_\mu \partial^\nu] = 0, \tag{5.154}$$

but this is an identity which is solved for every value of the momentum. Thus, the Green function in eqn. (5.151) supplies an infinite number of solutions for A_μ for every J , one for each unrestricted value of k , which makes eqn. (5.151) singular.

The problem can be traced to the gauge symmetry of the field $A_\mu(x)$. Under a gauge transformation, $A_\mu \rightarrow A_\mu + \partial_\mu s$, but

$$[-\square \delta_\mu^\nu + \partial_\mu \partial^\nu] (\partial_\nu s) = 0 \tag{5.155}$$

¹⁰Note that the operator has one index up and one index down, thereby mapping contravariant eigenvectors to contravariant eigenvectors

for any function $s(x)$. It can be circumvented by breaking the gauge symmetry in such a way that the integral over k in eqn. (5.151) is restricted. A convenient choice is the so-called Lorentz gauge condition

$$\partial_\mu A^\mu = 0. \quad (5.156)$$

This can be enforced by adding a Lagrange multiplier to the Maxwell action,

$$S \rightarrow \int (dx) \left\{ \frac{1}{4\mu_0} F^{\mu\nu} F_{\mu\nu} - J^\mu A_\mu + \frac{1}{2\alpha} \mu_0^{-1} (\partial^\mu A_\mu)^2 \right\}, \quad (5.157)$$

so that eqn. (5.149) is modified to

$$\left[-\square \delta_\mu^v + \left(1 - \frac{1}{\alpha} \right) \partial_\mu \partial^v \right] A^\mu(x) = J^v. \quad (5.158)$$

It may now be verified that the determinant of the operator no longer vanishes for all α ; thus, a formal constraint is implied over the k_μ , and the Green function may be written

$$D_{\mu\nu}(x, x') = c\mu_0 \int (dk) e^{ik(x-x')} \left[\frac{g_{\mu\nu}}{k^2} + (\alpha - 1) \frac{k_\mu k_\nu}{k^4} \right]. \quad (5.159)$$

This constraint is not a complete breakage of the gauge symmetry, since one may gauge transform eqn. (5.156) and show that

$$\partial_\mu A^\mu \rightarrow \partial_\mu A^\mu + \square s(x) = 0. \quad (5.160)$$

Thus, the gauge condition still admits restricted gauge transformations such that

$$\square s(x) = 0. \quad (5.161)$$

However, this modification is sufficient to obtain a formal Green function, and so the additional gauge multi-valuedness is often not addressed.

5.8 Principal values and Kramers–Kronig relations

Green functions which satisfy retarded (or advanced) boundary conditions satisfy a special pair of Fourier frequency-space relations, called the Kramers–Kronig relations (these are also referred to as Bode's law in circuit theory), by virtue of the fact that all of their poles lie in one half-plane (see figure 5.5). These relations are an indication of purely causal or purely acausal behaviour. In particular, physical response functions satisfy such relations, including the refractive index (or susceptibility, in non-magnetic materials) and the conductivity.

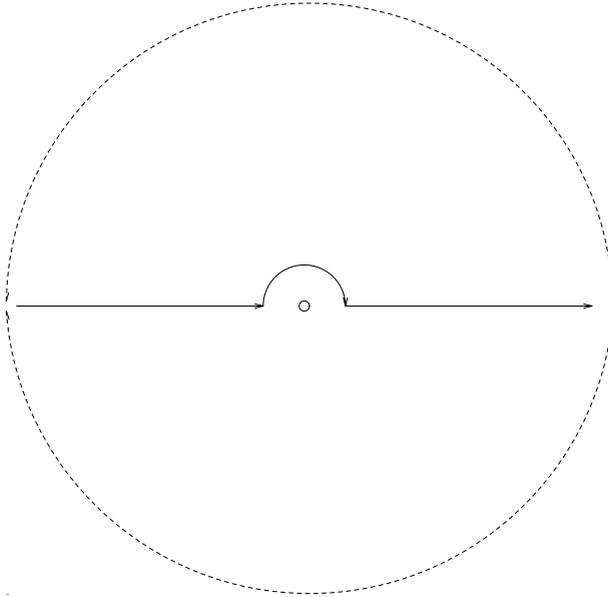


Fig. 5.5. Contour in the complex plane for the Kramers–Kronig relations.

Cauchy's integral formula states that the value of a function $G(\omega)$, which is analytic at every point within and on a closed curve C , and is evaluated at a point $\omega = z$, is given by the integral around the closed loop C of

$$\oint_C \frac{G(\omega)}{\omega - z} = 2\pi i G(z). \quad (5.162)$$

If a point P lies outside the closed loop, the value of the integral at that point is zero. Consider then a field $G(t - t')$ which satisfies retarded boundary conditions

$$G(t - t') = \int \frac{d\omega}{2\pi} e^{-i\omega(t-t')} G(\omega). \quad (5.163)$$

The Fourier transform $G(\omega)$, where

$$G(\omega) = \int d(t - t') e^{i\omega(t-t')} G(t - t') \quad (5.164)$$

is analytic in the upper half-plane, as in figure 5.5, but has a pole on the real axis. In the analytic upper region, the integral around a closed curve is zero, by Cauchy's theorem:

$$\oint_C \frac{G(\omega)d\omega}{\omega - z} = 0, \quad (5.165)$$

where we assume that $G(z)$ has a simple pole at $\omega = z$. We can write the parts of this integral in terms of the principal value of the integral along the real axis, plus the integral around the small semi-circle enclosing the pole. The integral over the semi-circle at infinity vanishes over the causal region, since $\exp(i\omega(t - t'))$ converges if $t - t' > 0$ and ω has a positive imaginary part. Around the semi-circle we have, letting $\omega - z = \epsilon e^{i\theta}$,

$$\begin{aligned} \oint_{SC} \frac{G(\omega)d\omega}{\omega - z} &= - \lim_{\epsilon \rightarrow 0} \int_0^\pi \frac{G(\epsilon e^{i\theta})i\epsilon e^{i\theta} d\theta}{\epsilon e^{i\theta}} \\ &= -i\pi (\epsilon e^{i\theta} + z) \Big|_{\epsilon \rightarrow 0} \\ &= -i\pi G(z). \end{aligned} \tag{5.166}$$

Then we have

$$\oint_C \frac{G(\omega)d\omega}{\omega - z} = P \int_{-\infty}^\infty \frac{G(\omega)d\omega}{\omega - z} - i\pi G(z) = 0. \tag{5.167}$$

The first term on the left hand side is the so-called *principal value* of the integral along the real axis. For a single pole, the principal value is defined strictly by the limit

$$P \int_{-\infty}^{+\infty} \equiv \lim_{\epsilon \rightarrow 0} \left\{ \int_{-\infty}^{p_i - \epsilon} + \int_{p_i + \epsilon}^\infty \right\}, \tag{5.168}$$

which approaches the singularity from equal distances on both sides. The expression may be generalized to two or more poles by arranging the limits of the integral to approach all poles symmetrically. Thus, if we now write the real and imaginary parts of $G(\omega)$ explicitly as

$$G(z) \equiv G_R(z) + iG_I(z), \tag{5.169}$$

and substitute this into eqn. (5.167), then, comparing real and imaginary parts we have:

$$\begin{aligned} P \int_{-\infty}^\infty \frac{G_R(\omega)d\omega}{\omega - z} &= -\pi G_I(z) \\ P \int_{-\infty}^\infty \frac{G_I(\omega)d\omega}{\omega - z} &= \pi G_R(z). \end{aligned} \tag{5.170}$$

These are the so-called Kramers–Kronig relations. They indicate that the analyticity of $G(t - t')$ implies a relationship between the real and imaginary parts of $G(t - t')$.

The generalization of these expressions to several poles along the real axis may be written

$$P \int_{-\infty}^\infty \frac{G_{I/R}(\omega)d\omega}{\omega - z} = \sum_{\text{poles}} \pm \pi G_{R/I}(z). \tag{5.171}$$

The integral along the real axis piece of the contour may be used to derive an expression for the principal value of $1/\omega$. From eqn. (5.167), we may write

$$\frac{1}{\omega - z} = P \frac{1}{\omega - z} - i\pi \delta(\omega - z). \quad (5.172)$$

This relation assumes that we have integrated along the real axis in a positive direction, avoiding a single pole on the real axis by passing *above* it (or, equivalently, by pushing the pole into the lower half-plane by an infinitesimal amount $i\epsilon$). Apart from these assumptions, it is quite general. It does not make any other assumptions about the nature of $G(\omega)$, nor does it depend on the presence of any other poles which do not lie on the real axis. It is a property of the special contour segment which passes around one pole. Had the contour passed under the pole instead of over it, the sign of the second term would have been changed. These results can be summarized and generalized to several poles on the real axis, by writing

$$\frac{1}{\omega - z \pm i\epsilon_j} = P \frac{1}{\omega - z} \mp \sum_j i\pi \delta(\omega - z_j), \quad (5.173)$$

where z is a general point in the complex plane, z_j are the poles on the real axis and $\epsilon \rightarrow 0$ is assumed. The upper sign is that for passing over the poles, while the lower sign is for passing under.

5.9 Representation of bound states in field theory

Bound states are states in which ‘particles’ are completely confined by a potential $V(x)$. Confinement is a simple interaction between two different fields: a dynamical field $\psi(x)$ and a static confining field $V(x)$. The way in which one represents bound states in field theory depends on which properties are germane to the description of the physical system. There are two possibilities.

The first alternative is the approach traditionally used in quantum mechanics. Here one considers the potential $V(x)$ to be a fixed potential, which breaks translational symmetry, e.g.

$$\left(-\frac{\hbar^2}{2m} \nabla^2 + V(\mathbf{x}) \right) \psi(x) = i\partial_t \psi(x). \quad (5.174)$$

One then considers the equation of motion of $\psi(x)$ in the rest frame of this potential and solves it using whatever methods are available. A Green function formulation of this problem leads to the Lippman–Schwinger equation for example (see section 17.5). In this case, the dynamical variable is the field, which moves in an external potential and is confined by it, e.g. electrons moving in the spherical hydrogen atom potential.

A second possibility is to consider bound states as multi-level, internal properties of the dynamical variables in question. For instance, instead of formulating the motion of electrons in a hydrogen atom, one formulates the motion of hydrogen atoms with internal electron levels which can be excited. To do this, one introduces multiplet states (an index A on the field and on the constant potential), e.g.

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + V_A\right)\psi_A(x) = i\partial_t\psi_A(x). \quad (5.175)$$

This is an effective theory in which one takes the average value of the potential V_A at N different levels, where $A = 1, \dots, N$. The values of V_A signify the energy differences between levels in the atom. The field ψ_A now represents the whole atom, not the electron within in. Clearly, all the components of ψ_A move together, according to the same equation of motion. The internal indices have the character of a broken internal ‘symmetry’. This approach allows one to study the dynamics and kinematics of hydrogen atoms in motion (rather than the behaviour of electrons in the rest frame of the atom). Such a study is of interest when considering how transitions are affected by sources outside the atom. An example of this is provided by the classic interaction between two levels of a neutral atom and an external radiation field (see section 10.6.3). This approach is applicable to laser cooling, for instance, where radiation momentum has a breaking effect on the kinetic activity of the atoms.