

# Chapter 5

## Green Functions

In this chapter we will study strategies for solving the inhomogeneous linear differential equation  $Ly = f$ . The tool we use is the *Green function*, which is an integral kernel representing the inverse operator  $L^{-1}$ . Apart from their use in solving inhomogeneous equations, Green functions play an important role in many areas of physics.

### 5.1 Inhomogeneous linear equations

We wish to solve  $Ly = f$  for  $y$ . Before we set about doing this, we should ask ourselves whether a solution *exists*, and, if it does, whether it is *unique*. The answers to these questions are summarized by the *Fredholm alternative*.

#### 5.1.1 Fredholm alternative

The Fredholm alternative for operators on a finite-dimensional vector space is discussed in detail in the appendix on linear algebra. You will want to make sure that you have read and understood this material. Here, we merely restate the results.

Let  $V$  be finite-dimensional vector space equipped with an inner product, and let  $A$  be a linear operator  $A : V \rightarrow V$  on this space. Then

**I. Either**

i)  $Ax = b$  has a *unique* solution,

**or**

ii)  $Ax = 0$  has a non-trivial solution.

- II. If  $Ax = 0$  has  $n$  linearly independent solutions, then so does  $A^\dagger x = 0$ .  
 III. If alternative ii) holds, then  $Ax = b$  has *no* solution unless  $b$  is perpendicular to all solutions of  $A^\dagger x = 0$ .

What is important for us in the present chapter is that this result continues to hold for linear differential operators  $L$  on a finite interval — provided that we define  $L^\dagger$  as in the previous chapter, *and provided the number of boundary conditions is equal to the order of the equation*.

If the number of boundary conditions is *not* equal to the order of the equation then the number of solutions to  $Ly = 0$  and  $L^\dagger y = 0$  will differ in general. It is still true, however, that  $Ly = f$  has *no* solution unless  $f$  is perpendicular to all solutions of  $L^\dagger y = 0$ .

*Example:* As an illustration of what happens when an equation with too many boundary conditions, consider

$$Ly = \frac{dy}{dx}, \quad y(0) = y(1) = 0. \quad (5.1)$$

Clearly  $Ly = 0$  has only the trivial solution  $y \equiv 0$ . If a solution to  $Ly = f$  exists, therefore, it will be unique.

We know that  $L^\dagger = -d/dx$ , with *no* boundary conditions on the functions in its domain. The equation  $L^\dagger y = 0$  therefore has the non-trivial solution  $y = 1$ . This means that there should be no solution to  $Ly = f$  unless

$$\langle 1, f \rangle = \int_0^1 f dx = 0. \quad (5.2)$$

If this condition is satisfied then

$$y(x) = \int_0^x f(x) dx \quad (5.3)$$

satisfies both the differential equation and the boundary conditions at  $x = 0, 1$ . If the condition is not satisfied,  $y(x)$  is not a solution, because  $y(1) \neq 0$ .

Initially we only solve  $Ly = f$  for homogeneous boundary conditions. After we have understood how to do this, we will extend our methods to deal with differential equations with inhomogeneous boundary conditions.

## 5.2 Constructing Green functions

We will solve  $Ly = f$ , a differential equation with homogeneous boundary conditions, by finding an inverse operator  $L^{-1}$ , so that  $y = L^{-1}f$ . This

inverse operator  $L^{-1}$  will be represented by an integral kernel

$$(L^{-1})_{x,\xi} = G(x, \xi), \quad (5.4)$$

with the property

$$L_x G(x, \xi) = \delta(x - \xi). \quad (5.5)$$

Here, the subscript  $x$  on  $L$  indicates that  $L$  acts on the first argument,  $x$ , of  $G$ . Then

$$y(x) = \int G(x, \xi) f(\xi) d\xi \quad (5.6)$$

will obey

$$L_x y = \int L_x G(x, \xi) f(\xi) d\xi = \int \delta(x - \xi) f(\xi) d\xi = f(x). \quad (5.7)$$

The problem is how to construct  $G(x, \xi)$ . There are three necessary ingredients:

- the function  $\chi(x) \equiv G(x, \xi)$  must have some discontinuous behaviour at  $x = \xi$  in order to generate the delta function;
- away from  $x = \xi$ , the function  $\chi(x)$  must obey  $L\chi = 0$ ;
- the function  $\chi(x)$  must obey the homogeneous boundary conditions required of  $y$  at the ends of the interval.

The last ingredient ensures that the resulting solution,  $y(x)$ , obeys the boundary conditions. It also ensures that the range of the integral operator  $G$  lies within the domain of  $L$ , a prerequisite if the product  $LG = I$  is to make sense. The manner in which these ingredients are assembled to construct  $G(x, \xi)$  is best explained through examples.

### 5.2.1 Sturm-Liouville equation

We begin by constructing the solution to the equation

$$(p(x)y')' + q(x)y(x) = f(x) \quad (5.8)$$

on the finite interval  $[a, b]$  with homogeneous self-adjoint boundary conditions

$$\frac{y'(a)}{y(a)} = \tan \theta_L, \quad \frac{y'(b)}{y(b)} = \tan \theta_R. \quad (5.9)$$

We therefore seek a function  $G(x, \xi)$  such that  $\chi(x) = G(x, \xi)$  obeys

$$L\chi = (p\chi)' + q\chi = \delta(x - \xi), \quad (5.10)$$

The function  $\chi(x)$  must also obey the homogeneous boundary conditions we require of  $y(x)$ .

Now (5.10) tells us that  $\chi(x)$  must be continuous at  $x = \xi$ . For if not, the two differentiations applied to a jump function would give us the derivative of a delta function, and we want only a plain  $\delta(x - \xi)$ . If we write

$$G(x, \xi) = \chi(x) = \begin{cases} Ay_L(x)y_R(\xi), & x < \xi, \\ Ay_L(\xi)y_R(x), & x > \xi, \end{cases} \quad (5.11)$$

then  $\chi(x)$  is automatically continuous at  $x = \xi$ . We take  $y_L(x)$  to be a solution of  $Ly = 0$ , chosen to satisfy the boundary condition at the left hand end of the interval. Similarly  $y_R(x)$  should solve  $Ly = 0$  and satisfy the boundary condition at the right hand end. With these choices we satisfy (5.10) at all points away from  $x = \xi$ .

To work out how to satisfy the equation exactly *at* the location of the delta-function, we integrate (5.10) from  $\xi - \varepsilon$  to  $\xi + \varepsilon$  and find that

$$p(\xi)[\chi'(\xi + \varepsilon) - \chi'(\xi - \varepsilon)] = 1 \quad (5.12)$$

With our product form for  $\chi(x)$ , this *jump condition* becomes

$$Ap(\xi)\left(y_L(\xi)y_R'(\xi) - y_L'(\xi)y_R(\xi)\right) = 1 \quad (5.13)$$

and determines the constant  $A$ . We recognize the Wronskian  $W(y_L, y_R; \xi)$  on the left hand side of this equation. We therefore have  $A = 1/(pW)$  and

$$G(x, \xi) = \begin{cases} \frac{1}{pW}y_L(x)y_R(\xi), & x < \xi, \\ \frac{1}{pW}y_L(\xi)y_R(x), & x > \xi. \end{cases} \quad (5.14)$$

For the Sturm-Liouville equation the product  $pW$  is constant. This fact follows from Liouville's formula,

$$W(x) = W(0) \exp\left\{-\int_0^x \left(\frac{p_1}{p_0}\right) d\xi\right\}, \quad (5.15)$$

and from  $p_1 = p_0' = p'$  in the Sturm-Liouville equation. Thus

$$W(x) = W(0) \exp\left(-\ln[p(x)/p(0)]\right) = W(0) \frac{p(0)}{p(x)}. \quad (5.16)$$

The constancy of  $pW$  means that  $G(x, \xi)$  is symmetric:

$$G(x, \xi) = G(\xi, x). \quad (5.17)$$

This is as it should be. The inverse of a symmetric matrix (and the real, self-adjoint, Sturm-Liouville operator is the function-space analogue of a real symmetric matrix) is itself symmetric.

The solution to

$$Ly = (p_0 y')' + qy = f(x) \quad (5.18)$$

is therefore

$$y(x) = \frac{1}{Wp} \left\{ y_L(x) \int_x^b y_R(\xi) f(\xi) d\xi + y_R(x) \int_a^x y_L(\xi) f(\xi) d\xi \right\}. \quad (5.19)$$

Take care to understand the ranges of integration in this formula. In the first integral  $\xi > x$  and we use  $G(x, \xi) \propto y_L(x)y_R(\xi)$ . In the second integral  $\xi < x$  and we use  $G(x, \xi) \propto y_L(\xi)y_R(x)$ . It is easy to get these the wrong way round.

Because we must divide by it in constructing  $G(x, \xi)$ , it is necessary that the Wronskian  $W(y_L, y_R)$  not be zero. This is reasonable. If  $W$  were zero then  $y_L \propto y_R$ , and the single function  $y_R$  satisfies both  $Ly_R = 0$  and the boundary conditions. This means that the differential operator  $L$  has  $y_R$  as a zero-mode, so there can be no unique solution to  $Ly = f$ .

*Example:* Solve

$$-\partial_x^2 y = f(x), \quad y(0) = y(1) = 0. \quad (5.20)$$

We have

$$\left. \begin{array}{l} y_L = x \\ y_R = 1 - x \end{array} \right\} \Rightarrow y'_L y_R - y_L y'_R \equiv 1. \quad (5.21)$$

We find that

$$G(x, \xi) = \begin{cases} x(1 - \xi), & x < \xi, \\ \xi(1 - x), & x > \xi, \end{cases} \quad (5.22)$$

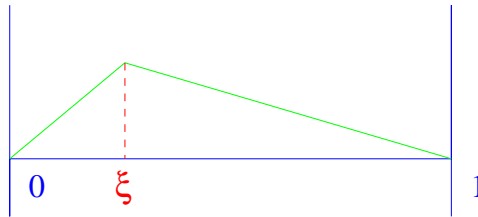


Figure 5.1: The function  $\chi(x) = G(x, \xi)$ .

and

$$y(x) = (1-x) \int_0^x \xi f(\xi) d\xi + x \int_x^1 (1-\xi) f(\xi) d\xi. \quad (5.23)$$

### 5.2.2 Initial-value problems

*Initial value* problems are those boundary-value problems where all boundary conditions are imposed at one end of the interval, instead of some conditions at one end and some at the other. The same ingredients go into to constructing the Green function, though.

Consider the problem

$$\frac{dy}{dt} - Q(t)y = F(t), \quad y(0) = 0. \quad (5.24)$$

We seek a Green function such that

$$L_t G(t, t') \equiv \left( \frac{d}{dt} - Q(t) \right) G(t, t') = \delta(t - t') \quad (5.25)$$

and  $G(0, t') = 0$ .

We need  $\chi(t) = G(t, t')$  to satisfy  $L_t \chi = 0$ , except at  $t = t'$ , and need  $\chi(0) = 0$ . The unique solution of  $L_t \chi = 0$  with  $\chi(0) = 0$  is  $\chi(t) \equiv 0$ . This means that  $G(t, 0) = 0$  for all  $t < t'$ . Near  $t = t'$  we have the jump condition

$$G(t' + \varepsilon, t') - G(t' - \varepsilon, t') = 1. \quad (5.26)$$

The unique solution is

$$G(t, t') = \theta(t - t') \exp \left\{ \int_{t'}^t Q(s) ds \right\}, \quad (5.27)$$

where  $\theta(t - t')$  is the Heaviside step distribution

$$\theta(t) = \begin{cases} 0, & t < 0, \\ 1, & t > 0. \end{cases} \quad (5.28)$$

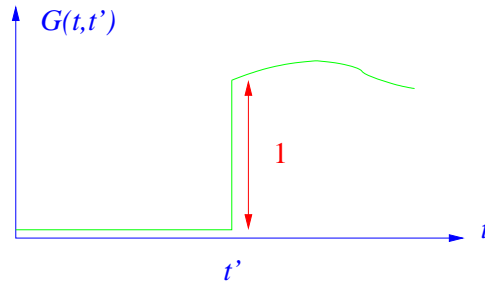


Figure 5.2: The Green function  $G(t, t')$  for the first-order initial value problem

Therefore

$$\begin{aligned}
 y(t) &= \int_0^\infty G(t, t')F(t')dt', \\
 &= \int_0^t \exp\left\{\int_{t'}^t Q(s) ds\right\} F(t') dt' \\
 &= \exp\left\{\int_0^t Q(s) ds\right\} \int_0^t \exp\left\{-\int_0^{t'} Q(s) ds\right\} F(t') dt'. \quad (5.29)
 \end{aligned}$$

We earlier obtained this solution *via* variation of parameters.

*Example: Forced, Damped, Harmonic Oscillator.* An oscillator obeys the equation

$$\ddot{x} + 2\gamma\dot{x} + (\Omega^2 + \gamma^2)x = F(t). \quad (5.30)$$

Here  $\gamma > 0$  is the friction coefficient. Assuming that the oscillator is at rest at the origin at  $t = 0$ , we will show that

$$x(t) = \left(\frac{1}{\Omega}\right) \int_0^t e^{-\gamma(t-\tau)} \sin \Omega(t-\tau) F(\tau) d\tau. \quad (5.31)$$

We seek a Green function  $G(t, \tau)$  such that  $\chi(t) = G(t, \tau)$  obeys  $\chi(0) = \chi'(0) = 0$ . Again, the unique solution of the differential equation with this initial data is  $\chi(t) \equiv 0$ . The Green function must be continuous at  $t = \tau$ , but its derivative must be discontinuous there, jumping from zero to unity to provide the delta function. Thereafter, it must satisfy the homogeneous equation. The unique function satisfying all these requirements is

$$G(t, \tau) = \theta(t - \tau) \frac{1}{\Omega} e^{-\gamma(t-\tau)} \sin \Omega(t - \tau). \quad (5.32)$$

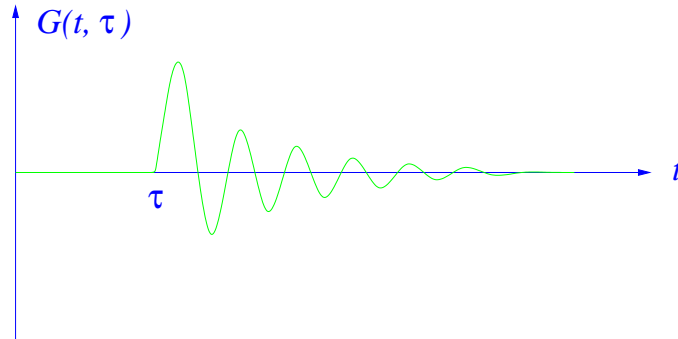


Figure 5.3: *The Green function  $G(t, \tau)$  for the damped oscillator problem .*

Both these initial-value Green functions  $G(t, t')$  are identically zero when  $t < t'$ . This is because the Green function is the response of the system to a kick at time  $t = t'$ , and in physical problems no effect comes before its cause. Such Green functions are said to be *causal*.

**Physics application: friction without friction—the Caldeira-Leggett model in real time.**

We now describe an application of the initial-value problem Green function we found in the preceding example.

When studying the quantum mechanics of systems with friction, such as the viscously damped oscillator, we need a tractable model of the dissipative process. Such a model was introduced by Caldeira and Leggett.<sup>1</sup> They consider the Lagrangian

$$L = \frac{1}{2} \left( \dot{Q}^2 - (\Omega^2 - \Delta\Omega^2)Q^2 \right) - Q \sum_i f_i q_i + \sum_i \frac{1}{2} (\dot{q}_i^2 - \omega_i^2 q_i^2), \quad (5.33)$$

which describes a macroscopic variable  $Q(t)$ , linearly coupled to an *oscillator bath* of very many simple systems  $q_i$  representing the environment. The quantity

$$\Delta\Omega^2 \stackrel{\text{def}}{=} - \sum_i \left( \frac{f_i^2}{\omega_i^2} \right), \quad (5.34)$$

<sup>1</sup>A. Caldeira, A. J. Leggett, *Phys. Rev. Lett.* **46** (1981) 211.



is a counter-term that is inserted cancel the frequency shift

$$\Omega^2 \rightarrow \Omega^2 - \sum_i \left( \frac{f_i^2}{\omega_i^2} \right), \quad (5.35)$$

caused by the coupling to the bath.<sup>2</sup>

The equations of motion are

$$\begin{aligned} \ddot{Q} + (\Omega^2 - \Delta\Omega^2)Q + \sum_i f_i q_i &= 0, \\ \ddot{q}_i + \omega_i^2 q_i + f_i Q &= 0. \end{aligned} \quad (5.36)$$

Using our initial-value Green function, we solve for the  $q_i$  in terms of  $Q(t)$ :

$$f_i q_i = - \int_{-\infty}^t \left( \frac{f_i^2}{\omega_i} \right) \sin \omega_i(t - \tau) Q(\tau) d\tau. \quad (5.37)$$

The resulting motion of the  $q_i$  feeds back into the equation for  $Q$  to give

$$\ddot{Q} + (\Omega^2 - \Delta\Omega^2)Q + \int_{-\infty}^t F(t - \tau) Q(\tau) d\tau = 0, \quad (5.38)$$

where

$$F(t) \stackrel{\text{def}}{=} - \sum_i \left( \frac{f_i^2}{\omega_i} \right) \sin(\omega_i t) \quad (5.39)$$

is a *memory function*.

It is now convenient to introduce a *spectral function*

$$J(\omega) \stackrel{\text{def}}{=} \frac{\pi}{2} \sum_i \left( \frac{f_i^2}{\omega_i} \right) \delta(\omega - \omega_i), \quad (5.40)$$

which characterizes the spectrum of couplings and frequencies associated with the oscillator bath. In terms of  $J(\omega)$  we can write

$$F(t) = -\frac{2}{\pi} \int_0^\infty J(\omega) \sin(\omega t) d\omega. \quad (5.41)$$

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<sup>2</sup>The shift arises because a static  $Q$  displaces the bath oscillators so that  $f_i q_i = -(f_i^2/\omega_i^2)Q$ . Substituting these values for the  $f_i q_i$  into the potential terms shows that, in the absence of  $\Delta\Omega^2 Q^2$ , the effective potential seen by  $Q$  would be

$$\frac{1}{2}\Omega^2 Q^2 + Q \sum_i f_i q_i + \sum_i \frac{1}{2}\omega_i^2 q_i^2 = \frac{1}{2} \left( \Omega^2 - \sum_i \left( \frac{f_i^2}{\omega_i^2} \right) \right) Q^2.$$

Although  $J(\omega)$  is defined as a sum of delta function “spikes,” the oscillator bath contains a very large number of systems and this makes  $J(\omega)$  effectively a smooth function. This is just as the density of a gas (a sum of delta functions at the location of the atoms) is macroscopically smooth. By taking different forms for  $J(\omega)$  we can represent a wide range of environments. Caldeira and Leggett show that to obtain a friction force proportional to  $\dot{Q}$  we should make  $J(\omega)$  proportional to the frequency  $\omega$ . To see how this works, consider the choice

$$J(\omega) = \eta\omega \left[ \frac{\Lambda^2}{\Lambda^2 + \omega^2} \right], \quad (5.42)$$

which is equal to  $\eta\omega$  for small  $\omega$ , but tends to zero when  $\omega \gg \Lambda$ . The high-frequency cutoff  $\Lambda$  is introduced to make the integrals over  $\omega$  converge. With this cutoff

$$\frac{2}{\pi} \int_0^\infty J(\omega) \sin(\omega t) d\omega = \frac{2}{2\pi i} \int_{-\infty}^\infty \frac{\eta\omega\Lambda^2 e^{i\omega t}}{\Lambda^2 + \omega^2} d\omega = \text{sgn}(t)\eta\Lambda^2 e^{-\Lambda|t|}. \quad (5.43)$$

Therefore,

$$\begin{aligned} \int_{-\infty}^t F(t-\tau)Q(\tau) d\tau &= - \int_{-\infty}^t \eta\Lambda^2 e^{-\Lambda|t-\tau|} Q(\tau) d\tau \\ &= -\eta\Lambda Q(t) + \eta\dot{Q}(t) - \frac{\eta}{2\Lambda}\ddot{Q}(t) + \dots, \end{aligned} \quad (5.44)$$

where the second line results from expanding  $Q(\tau)$  as a Taylor series

$$Q(\tau) = Q(t) + (\tau - t)\dot{Q}(t) + \dots, \quad (5.45)$$

and integrating term-by-term. Now,

$$-\Delta\Omega^2 \equiv \sum_i \left( \frac{f_i^2}{\omega_i^2} \right) = \frac{2}{\pi} \int_0^\infty \frac{J(\omega)}{\omega} d\omega = \frac{2}{\pi} \int_0^\infty \frac{\eta\Lambda^2}{\Lambda^2 + \omega^2} d\omega = \eta\Lambda. \quad (5.46)$$

The  $-\Delta\Omega^2 Q$  counter-term thus cancels the leading term  $-\eta\Lambda Q(t)$  in (5.44), which would otherwise represent a  $\Lambda$ -dependent frequency shift. After this cancellation we can safely let  $\Lambda \rightarrow \infty$ , and so ignore terms with negative powers of the cutoff. The only surviving term in (5.44) is then  $\eta\dot{Q}$ . This we substitute into (5.38), which becomes the equation for viscously damped motion:

$$\ddot{Q} + \eta\dot{Q} + \Omega^2 Q = 0. \quad (5.47)$$

The oscillators in the bath absorb energy but, unlike a pair of coupled oscillators which trade energy rhythmically back-and-forth, the incommensurate motion of the many  $q_i$  prevents them from cooperating for long enough to return any energy to  $Q(t)$ .

### 5.2.3 Modified Green function

When the equation  $Ly = 0$  has a non trivial-solution, there can be no unique solution to  $Ly = f$ , but there still will be solutions provided  $f$  is orthogonal to all solutions of  $L^\dagger y = 0$ .

*Example:* Consider

$$Ly \equiv -\partial_x^2 y = f(x), \quad y'(0) = y'(1) = 0. \quad (5.48)$$

The equation  $Ly = 0$  has one non-trivial solution,  $y(x) = 1$ . The operator  $L$  is self-adjoint,  $L^\dagger = L$ , and so there will be solutions to  $Ly = f$  provided  $\langle 1, f \rangle = \int_0^1 f dx = 0$ .

We cannot define the the green function as a solution to

$$-\partial_x^2 G(x, \xi) = \delta(x - \xi), \quad (5.49)$$

because  $\int_0^1 \delta(x - \xi) dx = 1 \neq 0$ , but we can seek a solution to

$$-\partial_x^2 G(x, \xi) = \delta(x - \xi) - 1 \quad (5.50)$$

as the right-hand integrates to zero.

A general solution to  $-\partial_x^2 y = -1$  is

$$y = A + Bx + \frac{1}{2}x^2, \quad (5.51)$$

and the functions

$$\begin{aligned} y_L &= A + \frac{1}{2}x^2, \\ y_R &= C - x + \frac{1}{2}x^2, \end{aligned} \quad (5.52)$$

obey the boundary conditions at the left and right ends of the interval, respectively. Continuity at  $x = \xi$  demands that  $A = C - \xi$ , and we are left with

$$G(x, \xi) = \begin{cases} C - \xi + \frac{1}{2}x^2, & 0 < x < \xi \\ C - x + \frac{1}{2}x^2, & \xi < x < 1, \end{cases} \quad (5.53)$$

There is no freedom left to impose the condition

$$G'(\xi - \varepsilon, \xi) - G'(\xi + \varepsilon, \xi) = 1, \quad (5.54)$$

but it is *automatically satisfied!* Indeed,

$$\begin{aligned} G'(\xi - \varepsilon, \xi) &= \xi \\ G'(\xi + \varepsilon, \xi) &= -1 + \xi. \end{aligned} \quad (5.55)$$

We may select a different value of  $C$  for each  $\xi$ , and a convenient choice is

$$C = \frac{1}{2}\xi^2 + \frac{1}{3} \quad (5.56)$$

which makes  $G$  symmetric:

$$G(x, \xi) = \begin{cases} \frac{1}{3} - \xi + \frac{x^2 + \xi^2}{2}, & 0 < x < \xi \\ \frac{1}{3} - x + \frac{x^2 + \xi^2}{2}, & \xi < x < 1, \end{cases} \quad (5.57)$$

It also makes  $\int_0^1 G(x, \xi) dx = 0$ .

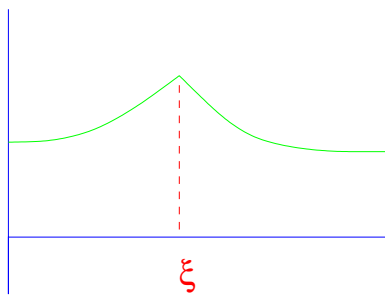


Figure 5.4: *The modified Green function.*

The solution to  $Ly = f$  is

$$y(x) = \int_0^1 G(x, \xi) f(\xi) d\xi + A, \quad (5.58)$$

where  $A$  is arbitrary.

## 5.3 Applications of Lagrange's identity

### 5.3.1 Hermiticity of Green functions

Earlier we noted the symmetry of the Green function for the Sturm-Liouville equation. We will now establish the corresponding result for general differential operators.

Let  $G(x, \xi)$  obey  $L_x G(x, \xi) = \delta(x - \xi)$  with homogeneous boundary conditions  $B$ , and let  $G^\dagger(x, \xi)$  obey  $L_x^\dagger G^\dagger(x, \xi) = \delta(x - \xi)$  with adjoint boundary conditions  $B^\dagger$ . Then, from Lagrange's identity, we have

$$\begin{aligned} [Q(G, G^\dagger)]_a^b &= \int_a^b dx \left\{ \left( L_x^\dagger G^\dagger(x, \xi) \right)^* G(x, \xi') - \left( G^\dagger(x, \xi) \right)^* L G(x, \xi') \right\} \\ &= \int_a^b dx \left\{ \delta(x - \xi) G(x, \xi') - \left( G^\dagger(x, \xi) \right)^* \delta(x - \xi') \right\} \\ &= G(\xi, \xi') - \left( G^\dagger(\xi', \xi) \right)^*. \end{aligned} \quad (5.59)$$

Thus, provided  $[Q(G, G^\dagger)]_a^b = 0$ , which is indeed the case because the boundary conditions for  $L$ ,  $L^\dagger$  are mutually adjoint, we have

$$G^\dagger(\xi, x) = \left( G(x, \xi) \right)^*, \quad (5.60)$$

and the Green functions, regarded as matrices with continuous rows and columns, are Hermitian conjugates of one another.

*Example:* Let

$$L = \frac{d}{dx}, \quad \mathcal{D}(L) = \{y, Ly \in L^2[0, 1] : y(0) = 0\}. \quad (5.61)$$

In this case  $G(x, \xi) = \theta(x - \xi)$ .

Now, we have

$$L^\dagger = -\frac{d}{dx}, \quad \mathcal{D}(L) = \{y, Ly \in L^2[0, 1] : y(1) = 0\} \quad (5.62)$$

and  $G^\dagger(x, \xi) = \theta(\xi - x)$ .

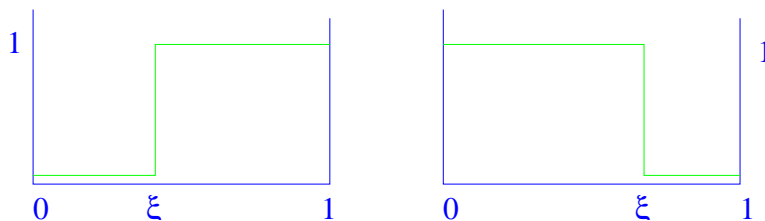


Figure 5.5:  $G(x, \xi) = \theta(x - \xi)$ , and  $G^\dagger(x, \xi) = \theta(\xi - x)$ .

### 5.3.2 Inhomogeneous boundary conditions

Our differential operators have been defined with linear *homogeneous* boundary conditions. We can, however, use them, and their Green-function inverses, to solve differential equations with *inhomogeneous* boundary conditions.

Suppose, for example, we wish to solve

$$-\partial_x^2 y = f(x), \quad y(0) = a, \quad y(1) = b. \quad (5.63)$$

We already know the Green function for the homogeneous boundary-condition problem with operator

$$L = -\partial_x^2, \quad \mathcal{D}(L) = \{y, Ly \in L^2[0, 1] : y(0) = 0, y(1) = 0\}. \quad (5.64)$$

It is

$$G(x, \xi) = \begin{cases} x(1 - \xi), & x < \xi, \\ \xi(1 - x), & x > \xi. \end{cases} \quad (5.65)$$

Now we apply Lagrange's identity to  $\chi(x) = G(x, \xi)$  and  $y(x)$  to get

$$\int_0^1 dx \left\{ G(x, \xi) \left( -\partial_x^2 y(x) \right) - y(x) \left( -\partial_x^2 G(x, \xi) \right) \right\} = [G'(x, \xi)y(x) - G(x, \xi)y'(x)]_0^1. \quad (5.66)$$

Here, as usual,  $G'(x, \xi) = \partial_x G(x, \xi)$ . The integral is equal to

$$\int dx \{ G(x, \xi) f(x) - y(x) \delta(x - \xi) \} = \int G(x, \xi) f(x) dx - y(\xi), \quad (5.67)$$

whilst the integrated-out bit is

$$-(1 - \xi)y(0) - 0 y'(0) - \xi y(1) + 0 y'(1). \quad (5.68)$$

Therefore, we have

$$y(\xi) = \int G(x, \xi) f(x) dx + (1 - \xi)y(0) + \xi y(1). \quad (5.69)$$

Here the term with  $f(x)$  is the particular integral, whilst the remaining terms constitute the complementary function (obeying the differential equation without the source term) which serves to satisfy the boundary conditions. Observe that the arguments in  $G(x, \xi)$  are not in the usual order, but, in the present example, this does not matter because  $G$  is symmetric.

When the operator  $L$  is not self-adjoint, we need to distinguish between  $L$  and  $L^\dagger$ , and  $G$  and  $G^\dagger$ . We then apply Lagrange's identity to the unknown function  $u(x)$  and  $\chi(x) = G^\dagger(x, \xi)$ .

*Example:* We will use the Green-function method to solve the differential equation

$$\frac{du}{dx} = f(x), \quad x \in [0, 1], \quad u(0) = a. \quad (5.70)$$

We can, of course, write down the answer to this problem directly, but it is interesting to see how the general strategy produces the solution. We first find the Green function  $G(x, \xi)$  for the operator with the corresponding homogeneous boundary conditions. In the present case, this operator is

$$L = \partial_x, \quad \mathcal{D}(L) = \{u, Lu \in L^2[0, 1] : u(0) = 0\}, \quad (5.71)$$

and the appropriate Green function is  $G(x, \xi) = \theta(x - \xi)$ . From  $G$  we then read off the adjoint Green function as  $G^\dagger(x, \xi) = (G(\xi, x))^*$ . In the present example, we have  $G^\dagger(x, \xi) = \theta(\xi - x)$ . We now use Lagrange's identity in the form

$$\int_0^1 dx \left\{ (L_x^\dagger G^\dagger(x, \xi))^* u(x) - (G^\dagger(x, \xi))^* L_x u(x) \right\} = [Q(G^\dagger, u)]_0^1. \quad (5.72)$$

In all cases, the left hand side is equal to

$$\int_0^1 dx \left\{ \delta(x - \xi) u(x) - G^T(x, \xi) f(x) \right\}, \quad (5.73)$$

where  $T$  denotes transpose,  $G^T(x, \xi) = G(\xi, x)$ . The left hand side is therefore equal to

$$u(\xi) - \int_0^1 dx G(\xi, x) f(x). \quad (5.74)$$

The right hand side depends on the details of the problem. In the present case, the integrated out part is

$$[Q(G^\dagger, u)]_0^1 = - [G^T(x, \xi)u(x)]_0^1 = u(0). \quad (5.75)$$

At the last step we have used the specific form  $G^T(x, \xi) = \theta(\xi - x)$  to find that only the lower limit contributes. The end result is therefore the expected one:

$$u(y) = u(0) + \int_0^y f(x) dx. \quad (5.76)$$

Variations of this strategy enable us to solve any inhomogeneous boundary-value problem in terms of the Green function for the corresponding homogeneous boundary-value problem.

## 5.4 Eigenfunction expansions

Self-adjoint operators possess a complete set of eigenfunctions, and we can expand the Green function in terms of these. Let

$$L\varphi_n = \lambda_n\varphi_n. \quad (5.77)$$

Let us further suppose that none of the  $\lambda_n$  are zero. Then the Green function has the eigenfunction expansion

$$G(x, \xi) = \sum_n \frac{\varphi_n(x)\varphi_n^*(\xi)}{\lambda_n}. \quad (5.78)$$

That this is so follows from

$$\begin{aligned} L_x \left( \sum_n \frac{\varphi_n(x)\varphi_n^*(\xi)}{\lambda_n} \right) &= \sum_n \frac{(L_x\varphi_n(x))\varphi_n^*(\xi)}{\lambda_n} \\ &= \sum_n \frac{\lambda_n\varphi_n(x)\varphi_n^*(\xi)}{\lambda_n} \\ &= \sum_n \varphi_n(x)\varphi_n^*(\xi) \\ &= \delta(x - \xi). \end{aligned} \quad (5.79)$$



*Example:* : Consider our familiar exemplar

$$L = -\partial_x^2, \quad \mathcal{D}(L) = \{y, Ly \in L^2[0, 1] : y(0) = y(1) = 0\}, \quad (5.80)$$

for which

$$G(x, \xi) = \begin{cases} x(1 - \xi), & x < \xi, \\ \xi(1 - x), & x > \xi. \end{cases} \quad (5.81)$$

Computing the Fourier series shows that

$$G(x, \xi) = \sum_{n=1}^{\infty} \left( \frac{2}{n^2\pi^2} \right) \sin(n\pi x) \sin(n\pi\xi). \quad (5.82)$$

### Modified Green function

When one or more of the eigenvalues is zero, a modified Green function is obtained by simply omitting the corresponding terms from the series.

$$G_{\text{mod}}(x, \xi) = \sum_{\lambda_n \neq 0} \frac{\varphi_n(x)\varphi_n^*(\xi)}{\lambda_n}. \quad (5.83)$$

Then

$$L_x G_{\text{mod}}(x, \xi) = \delta(x - \xi) - \sum_{\lambda_n = 0} \varphi_n(x)\varphi_n^*(\xi). \quad (5.84)$$

We see that this  $G_{\text{mod}}$  is still hermitian, and, as a function of  $x$ , is orthogonal to the zero modes. These are the properties we elected when constructing the modified Green function in equation (5.57).

## 5.5 Analytic properties of Green functions

In this section we study the properties of Green functions considered as functions of a complex variable. Some of the formulæ are slightly easier to derive using contour integral methods, but these are not necessary and we will not use them here. The only complex-variable prerequisite is a familiarity with complex arithmetic and, in particular, knowledge of how to take the logarithm and the square root of a complex number.

### 5.5.1 Causality implies analyticity

Consider a Green function of the form  $G(t - \tau)$  and possessing the causal property that  $G(t - \tau) = 0$ , for  $t < \tau$ . If the improper integral defining its Fourier transform,

$$\tilde{G}(\omega) = \int_0^\infty e^{i\omega t} G(t) dt \stackrel{\text{def}}{=} \lim_{T \rightarrow \infty} \left\{ \int_0^T e^{i\omega t} G(t) dt \right\}, \quad (5.85)$$

converges for real  $\omega$ , it will converge even better when  $\omega$  has a positive imaginary part. Consequently  $\tilde{G}(\omega)$  will be a well-behaved function of the complex variable  $\omega$  everywhere in the upper half of the complex  $\omega$  plane. Indeed, it will be *analytic* there, meaning that its Taylor series expansion about any point actually converges to the function. For example, the Green function for the damped harmonic oscillator

$$G(t) = \begin{cases} \frac{1}{\Omega} e^{-\gamma t} \sin(\Omega t), & t > 0, \\ 0, & t < 0, \end{cases} \quad (5.86)$$

has Fourier transform

$$\tilde{G}(\omega) = \frac{1}{\Omega^2 - (\omega + i\gamma)^2}, \quad (5.87)$$

which is always finite in the upper half-plane, although it has *pole* singularities at  $\omega = -i\gamma \pm \Omega$  in the lower half-plane.

The only way that the Fourier transform  $\tilde{G}$  of a causal Green function can have a pole singularity in the upper half-plane is if  $G$  contains an exponential factor growing in time, in which case the system is *unstable* to perturbations (and the real-frequency Fourier transform does not exist). This observation is at the heart of the *Nyquist criterion* for the stability of linear electronic devices.

Inverting the Fourier transform, we have

$$G(t) = \int_{-\infty}^{\infty} \frac{1}{\Omega^2 - (\omega + i\gamma)^2} e^{-i\omega t} \frac{d\omega}{2\pi} = \theta(t) \frac{1}{\Omega} e^{-\gamma t} \sin(\Omega t). \quad (5.88)$$

It is perhaps surprising that this integral is identically zero if  $t < 0$ , and non-zero if  $t > 0$ . This is one of the places where contour integral methods might cast some light, but because we have confidence in the Fourier inversion formula, we know that it must be correct.

Remember that in deriving (5.88) we have explicitly assumed that the damping coefficient  $\gamma$  is positive. It is important to realize that reversing the sign of  $\gamma$  on the left-hand side of (5.88) does more than just change  $e^{-\gamma t} \rightarrow e^{\gamma t}$  on the right-hand side. Naïvely setting  $\gamma \rightarrow -\gamma$  on both sides of (5.88) gives an equation that cannot possibly be true. The left-hand side would be the Fourier transform of a smooth function, and the Riemann-Lebesgue lemma tells us that such a Fourier transform must become zero when  $|t| \rightarrow \infty$ . The right-hand side, to the contrary, would be a function whose oscillations grow without bound as  $t$  becomes large and positive.

To find the correct equation, observe that we can legitimately effect the sign-change  $\gamma \rightarrow -\gamma$  by first complex-conjugating the integral and then changing  $t$  to  $-t$ . Performing these two operations on both sides of (5.88) leads to

$$\int_{-\infty}^{\infty} \frac{1}{\Omega^2 - (\omega - i\gamma)^2} e^{-i\omega t} \frac{d\omega}{2\pi} = -\theta(-t) \frac{1}{\Omega} e^{\gamma t} \sin(\Omega t) \quad (5.89)$$

The new right-hand side represents an exponentially growing oscillation that is suddenly silenced by the kick at  $t = 0$ .

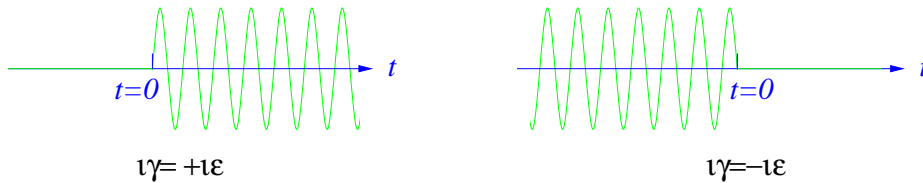


Figure 5.6: The effect on  $G(t)$ , the Green function of an undamped oscillator, of changing  $i\gamma$  from  $+i\varepsilon$  to  $-i\varepsilon$ .

The effect of taking the damping parameter  $\gamma$  from an infinitesimally small positive value  $\varepsilon$  to an infinitesimally small negative value  $-\varepsilon$  is therefore to turn the *causal* Green function (no motion before it is started by the delta-function kick) of the *undamped* oscillator into an *anti-causal* Green function (no motion after it is stopped by the kick). Ultimately, this is because the differential operator corresponding to a harmonic oscillator with *initial*-value data is not self-adjoint, and its adjoint operator corresponds to a harmonic oscillator with *final*-value data.

This discontinuous dependence on an infinitesimal damping parameter is the subject of the next few sections.

### Physics application: Caldeira-Leggett in frequency space

If we write the Caldeira-Leggett equations of motion (5.36) in Fourier frequency space by setting

$$Q(t) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} Q(\omega) e^{-i\omega t}, \quad (5.90)$$

and

$$q_i(t) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} q_i(\omega) e^{-i\omega t}, \quad (5.91)$$

we have (after including an external force  $F_{\text{ext}}$  to drive the system)

$$\begin{aligned} (-\omega^2 + (\Omega^2 - \Delta\Omega^2))Q(\omega) - \sum_i f_i q_i(\omega) &= F_{\text{ext}}(\omega), \\ (-\omega^2 + \omega_i^2)q_i(\omega) + f_i Q(\omega) &= 0. \end{aligned} \quad (5.92)$$

Eliminating the  $q_i$ , we obtain

$$\left(-\omega^2 + (\Omega^2 - \Delta\Omega^2)\right)Q(\omega) - \sum_i \frac{f_i^2}{\omega_i^2 - \omega^2} Q(\omega) = F_{\text{ext}}(\omega). \quad (5.93)$$

As before, sums over the index  $i$  are replaced by integrals over the spectral function

$$\sum_i \frac{f_i^2}{\omega_i^2 - \omega^2} \rightarrow \frac{2}{\pi} \int_0^{\infty} \frac{\omega' J(\omega')}{\omega'^2 - \omega^2} d\omega', \quad (5.94)$$

and

$$-\Delta\Omega^2 \equiv \sum_i \left(\frac{f_i^2}{\omega_i^2}\right) \rightarrow \frac{2}{\pi} \int_0^{\infty} \frac{J(\omega')}{\omega'} d\omega'. \quad (5.95)$$

Then

$$Q(\omega) = \left(\frac{1}{\Omega^2 - \omega^2 + \Pi(\omega)}\right) F_{\text{ext}}(\omega), \quad (5.96)$$

where the *self-energy*  $\Pi(\omega)$  is given by

$$\Pi(\omega) = \frac{2}{\pi} \int_0^{\infty} \left\{ \frac{J(\omega')}{\omega'} - \frac{\omega' J(\omega')}{\omega'^2 - \omega^2} \right\} d\omega' = -\omega^2 \frac{2}{\pi} \int_0^{\infty} \frac{J(\omega')}{\omega'(\omega'^2 - \omega^2)} d\omega'. \quad (5.97)$$

The expression

$$\mathcal{G}(\omega) \equiv \frac{1}{\Omega^2 - \omega^2 + \Pi(\omega)} \quad (5.98)$$

a typical *response function*. Analogous objects occur in all branches of physics.

For viscous damping we know that  $J(\omega) = \eta\omega$ . Let us evaluate the integral occurring in  $\Pi(\omega)$  for this case:

$$I(\omega) = \int_0^\infty \frac{d\omega'}{\omega'^2 - \omega^2}. \quad (5.99)$$

We will initially assume that  $\omega$  is positive. Now,

$$\frac{1}{\omega'^2 - \omega^2} = \frac{1}{2\omega} \left( \frac{1}{\omega' - \omega} - \frac{1}{\omega' + \omega} \right), \quad (5.100)$$

so

$$I(\omega) = \left[ \frac{1}{2\omega} \left( \ln(\omega' - \omega) - \ln(\omega' + \omega) \right) \right]_{\omega'=0}^\infty. \quad (5.101)$$

At the upper limit we have  $\ln \left( (\infty - \omega)/(\infty + \omega) \right) = \ln 1 = 0$ . The lower limit contributes

$$-\frac{1}{2\omega} \left( \ln(-\omega) - \ln(\omega) \right). \quad (5.102)$$

To evaluate the logarithm of a negative quantity we must use

$$\ln \omega = \ln |\omega| + i \arg \omega, \quad (5.103)$$

where we will take  $\arg \omega$  to lie in the range  $-\pi < \arg \omega < \pi$ .

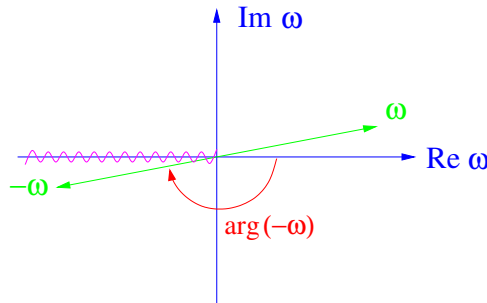


Figure 5.7: When  $\omega$  has a small positive imaginary part,  $\arg(-\omega) \approx -\pi$ .

To get an unambiguous answer, we need to give  $\omega$  an infinitesimal imaginary part  $\pm i\varepsilon$ . Depending on the sign of this imaginary part, we find that

$$I(\omega \pm i\varepsilon) = \pm \frac{i\pi}{2\omega}. \quad (5.104)$$

This formula remains true when the real part of  $\omega$  is negative, and so

$$\Pi(\omega \pm i\varepsilon) = \mp i\eta\omega. \quad (5.105)$$

Now the frequency-space version of

$$\ddot{Q}(t) + \eta\dot{Q} + \Omega^2 Q = F_{\text{ext}}(t) \quad (5.106)$$

is

$$(-\omega^2 - i\eta\omega + \Omega^2)Q(\omega) = F_{\text{ext}}(\omega), \quad (5.107)$$

so we must opt for the small shift in  $\omega$  that leads to  $\Pi(\omega) = -i\eta\omega$ . This means that we must regard  $\omega$  as having a *positive* infinitesimal imaginary part,  $\omega \rightarrow \omega + i\varepsilon$ . This imaginary part is a good and needful thing: it effects the replacement of the ill-defined singular integrals

$$G(t) \stackrel{?}{=} \int_0^\infty \frac{1}{\omega_i^2 - \omega^2} e^{-i\omega t} d\omega, \quad (5.108)$$

which arise as we transform back to real time, with the unambiguous expressions

$$G_\varepsilon(t) = \int_0^\infty \frac{1}{\omega_i^2 - (\omega + i\varepsilon)^2} e^{-i\omega t} d\omega. \quad (5.109)$$

The latter, we know, give rise to properly causal real-time Green functions.

### 5.5.2 Plemelj formulæ

The functions we are meeting can all be cast in the form

$$f(\omega) = \frac{1}{\pi} \int_a^b \frac{\rho(\omega')}{\omega' - \omega} d\omega'. \quad (5.110)$$

If  $\omega$  lies in the integration range  $[a, b]$ , then we divide by zero as we integrate over  $\omega' = \omega$ . We ought to avoid doing this, but this interval is often exactly where we desire to evaluate  $f$ . As before, we evade the division by zero by

giving  $\omega$  an infinitesimally small imaginary part:  $\omega \rightarrow \omega \pm i\varepsilon$ . We can then apply the *Plemelj formulæ*, named for the Slovenian mathematician Josip Plemelj, which say that

$$\begin{aligned} \frac{1}{2} \left( f(\omega + i\varepsilon) - f(\omega - i\varepsilon) \right) &= i\rho(\omega), \\ \frac{1}{2} \left( f(\omega + i\varepsilon) + f(\omega - i\varepsilon) \right) &= \frac{1}{\pi} P \int_{\Gamma} \frac{\rho(\omega')}{\omega' - \omega} d\omega'. \end{aligned} \quad (5.111)$$

As explained in section 2.3.2, the “*P*” in front of the integral stands for *principal part*. Recall that it means that we are to delete an infinitesimal segment of the  $\omega'$  integral lying symmetrically about the singular point  $\omega' = \omega$ .

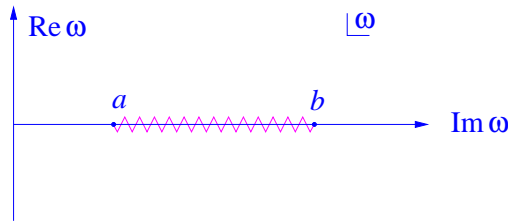


Figure 5.8: The analytic function  $f(\omega)$  is discontinuous across the real axis between  $a$  and  $b$ .

The Plemelj formula mean that the otherwise smooth and analytic function  $f(\omega)$  is discontinuous across the real axis between  $a$  and  $b$ . If the discontinuity  $\rho(\omega)$  is itself an analytic function then the line joining the points  $a$  and  $b$  is a *branch cut*, and the endpoints of the integral are *branch-point* singularities of  $f(\omega)$ .

The reason for the discontinuity may be understood by considering figure 5.9. The singular integrand is a product of  $\rho(\omega')$  with

$$\frac{1}{\omega' - (\omega \pm i\varepsilon)} = \frac{\omega' - \omega}{(\omega' - \omega)^2 + \varepsilon^2} \pm \frac{i\varepsilon}{(\omega' - \omega)^2 + \varepsilon^2}. \quad (5.112)$$

The first term on the right is a symmetrically cut-off version  $1/(\omega' - \omega)$  and provides the principal part integral. The the second term sharpens and tends to the delta function  $\pm i\pi\delta(\omega' - \omega)$  as  $\varepsilon \rightarrow 0$ , and so gives  $\pm i\pi\rho(\omega)$ . Because of this explanation, the Plemelj equations are commonly encoded in physics

papers via the “ $i\varepsilon$ ” cabbala

$$\frac{1}{\omega' - (\omega \pm i\varepsilon)} = P \left( \frac{1}{\omega' - \omega} \right) \pm i\pi\delta(\omega' - \omega). \quad (5.113)$$

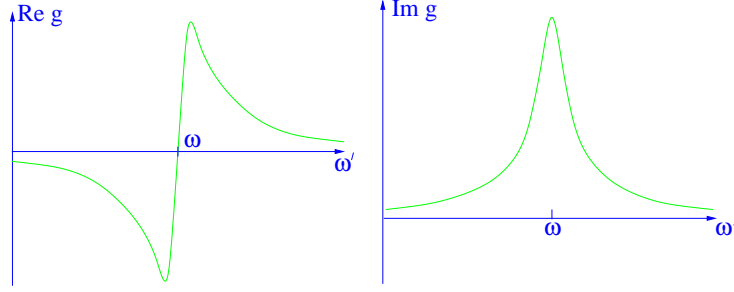


Figure 5.9: Sketch of the real and imaginary parts of  $g(\omega') = 1/(\omega' - (\omega + i\varepsilon))$ .

If  $\rho$  is real, as it often is, then  $f(\omega + i\eta) = (f(\omega - i\eta))^*$ . The discontinuity across the real axis is then purely imaginary, and

$$\frac{1}{2} \left( f(\omega + i\varepsilon) + f(\omega - i\varepsilon) \right) \quad (5.114)$$

is the real part of  $f$ . In this case we can write (5.110) as

$$\text{Re } f(\omega) = \frac{1}{\pi} P \int_a^b \frac{\text{Im } f(\omega')}{\omega' - \omega} d\omega'. \quad (5.115)$$

This formula is typical of the relations linking the real and imaginary parts of causal response functions.

A practical example of such a relation is provided by the complex, frequency-dependent, *refractive index*,  $n(\omega)$ , of a medium. This is defined so that a travelling electromagnetic wave takes the form

$$\mathbf{E}(x, t) = \mathbf{E}_0 e^{in(\omega)kx - i\omega t}. \quad (5.116)$$

Here,  $k = \omega/c$  is the *in vacuo* wavenumber. We can decompose  $n$  into its real and imaginary parts:

$$\begin{aligned} n(\omega) &= n_R + in_I \\ &= n_R(\omega) + \frac{i}{2|k|} \gamma(\omega), \end{aligned} \quad (5.117)$$



where  $\gamma$  is the extinction coefficient, defined so that the intensity falls off as  $I = I_0 \exp(-\gamma x)$ . A non-zero  $\gamma$  can arise from either energy absorption or scattering out of the forward direction. For the refractive index, the function  $f(\omega) = n(\omega) - 1$  can be written in the form of (5.110), and, using  $n(-\omega) = n^*(\omega)$ , this leads to the *Kramers-Kronig relation*

$$n_R(\omega) = 1 + \frac{c}{\pi} P \int_0^\infty \frac{\gamma(\omega')}{\omega'^2 - \omega^2} d\omega'. \quad (5.118)$$

Formulae like this will be rigorously derived in chapter 18 by the use of contour-integral methods.

### 5.5.3 Resolvent operator

Given a differential operator  $L$ , we define the *resolvent operator* to be  $R_\lambda \equiv (L - \lambda I)^{-1}$ . The resolvent is an analytic function of  $\lambda$ , except when  $\lambda$  lies in the spectrum of  $L$ .

We expand  $R_\lambda$  in terms of the eigenfunctions as

$$R_\lambda(x, \xi) = \sum_n \frac{\varphi_n(x) \varphi_n^*(\xi)}{\lambda_n - \lambda}. \quad (5.119)$$

When the spectrum is discrete, the resolvent has *poles* at the eigenvalues  $L$ . When the operator  $L$  has a continuous spectrum, the sum becomes an integral:

$$R_\lambda(x, \xi) = \int_{\mu \in \sigma(L)} \rho(\mu) \frac{\varphi_\mu(x) \varphi_\mu^*(\xi)}{\mu - \lambda} d\mu, \quad (5.120)$$

where  $\rho(\mu)$  is the eigenvalue density of states. This is of the form that we saw in connection with the Plemelj formulae. Consequently, when the spectrum comprises segments of the real axis, the resulting analytic function  $R_\lambda$  will be discontinuous across the real axis within them. The endpoints of the segments will branch point singularities of  $R_\lambda$ , and the segments themselves, considered as subsets of the complex plane, are the branch cuts.

The trace of the resolvent  $\text{Tr } R_\lambda$  is defined by

$$\begin{aligned} \text{Tr } R_\lambda &= \int dx \{R_\lambda(x, x)\} \\ &= \int dx \left\{ \sum_n \frac{\varphi_n(x) \varphi_n^*(x)}{\lambda_n - \lambda} \right\} \end{aligned}$$

$$\begin{aligned}
&= \sum_n \frac{1}{\lambda_n - \lambda} \\
&\rightarrow \int \frac{\rho(\mu)}{\mu - \lambda} d\mu.
\end{aligned} \tag{5.121}$$

Applying Plemelj to  $R_\lambda$ , we have

$$\operatorname{Im} \left[ \lim_{\varepsilon \rightarrow 0} \left\{ \operatorname{Tr} R_{\lambda+i\varepsilon} \right\} \right] = \pi \rho(\lambda). \tag{5.122}$$

Here, we have used that fact that  $\rho$  is real, so

$$\operatorname{Tr} R_{\lambda-i\varepsilon} = \left( \operatorname{Tr} R_{\lambda+i\varepsilon} \right)^*. \tag{5.123}$$

The non-zero imaginary part therefore shows that  $R_\lambda$  is discontinuous across the real axis at points lying in the continuous spectrum.

*Example:* Consider

$$L = -\partial_x^2 + m^2, \quad \mathcal{D}(L) = \{y, Ly \in L^2[-\infty, \infty]\}. \tag{5.124}$$

As we know, this operator has a continuous spectrum, with eigenfunctions

$$\varphi_k = \frac{1}{\sqrt{L}} e^{ikx}. \tag{5.125}$$

Here,  $L$  is the (very large) length of the interval. The eigenvalues are  $E = k^2 + m^2$ , so the spectrum is all positive numbers greater than  $m^2$ . The momentum density of states is

$$\rho(k) = \frac{L}{2\pi}. \tag{5.126}$$

The completeness relation is

$$\int_{-\infty}^{\infty} \frac{dk}{2\pi} e^{ik(x-\xi)} = \delta(x - \xi), \tag{5.127}$$

which is just the Fourier integral formula for the delta function.

The Green function for  $L$  is

$$G(x-y) = \int_{-\infty}^{\infty} dk \left( \frac{dn}{dk} \right) \frac{\varphi_k(x) \varphi_k^*(y)}{k^2 + m^2} = \int_{-\infty}^{\infty} \frac{dk}{2\pi} \frac{e^{ik(x-y)}}{k^2 + m^2} = \frac{1}{2m} e^{-m|x-y|}. \tag{5.128}$$

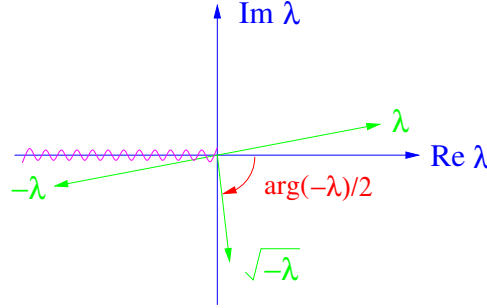


Figure 5.10: If  $\text{Im } \lambda > 0$ , and with the branch cut for  $\sqrt{z}$  in its usual place along the negative real axis, then  $\sqrt{-\lambda}$  has negative imaginary part and positive real part.

We can use the same calculation to look at the resolvent  $R_\lambda = (-\partial_x^2 - \lambda)^{-1}$ . Replacing  $m^2$  by  $-\lambda$ , we have

$$R_\lambda(x, y) = \frac{1}{2\sqrt{-\lambda}} e^{-\sqrt{-\lambda}|x-y|}. \quad (5.129)$$

To appreciate this expression, we need to know how to evaluate  $\sqrt{z}$  where  $z$  is complex. We write  $z = |z|e^{i\phi}$  where we require  $-\pi < \phi < \pi$ . We now define

$$\sqrt{z} = \sqrt{|z|}e^{i\phi/2}. \quad (5.130)$$

When we evaluate  $\sqrt{z}$  for  $z$  just below the negative real axis then this definition gives  $-i\sqrt{|z|}$ , and just above the axis we find  $+i\sqrt{|z|}$ . The discontinuity means that the negative real axis is a branch cut for the the square-root function. The  $\sqrt{-\lambda}$ 's appearing in  $R_\lambda$  therefore mean that the *positive* real axis will be a branch cut for  $R_\lambda$ . This branch cut therefore coincides with the spectrum of  $L$ , as promised earlier.

If  $\lambda$  is positive and we shift  $\lambda \rightarrow \lambda + i\varepsilon$  then

$$\frac{1}{2\sqrt{-\lambda}} e^{-\sqrt{-\lambda}|x-y|} \rightarrow \frac{i}{2\sqrt{\lambda}} e^{+i\sqrt{\lambda}|x-y| - \varepsilon|x-y|/2\sqrt{\lambda}}. \quad (5.131)$$

Notice that this decays away as  $|x-y| \rightarrow \infty$ . The square root retains a positive real part when  $\lambda$  is shifted to  $\lambda - i\varepsilon$ , and so the decay is still present:

$$\frac{1}{2\sqrt{-\lambda}} e^{-\sqrt{-\lambda}|x-y|} \rightarrow -\frac{i}{2\sqrt{\lambda}} e^{-i\sqrt{\lambda}|x-y| - \varepsilon|x-y|/2\sqrt{\lambda}}. \quad (5.132)$$

In each case, with  $\lambda$  either immediately above or immediately below the cut, the small imaginary part tempers the oscillatory behaviour of the Green function so that  $\chi(x) = G(x, y)$  is square integrable and remains an element of  $L^2[\mathbb{R}]$ .

We now take the trace of  $R$  by setting  $x = y$  and integrating:

$$\mathrm{Tr} R_{\lambda+i\varepsilon} = i\pi \frac{L}{2\pi\sqrt{|\lambda|}}. \quad (5.133)$$

Thus,

$$\rho(\lambda) = \theta(\lambda) \frac{L}{2\pi\sqrt{|\lambda|}}, \quad (5.134)$$

which coincides with our direct calculation.

*Example:* Let

$$L = -i\partial_x, \quad \mathcal{D}(L) = \{y, Ly \in L^2[\mathbb{R}]\}. \quad (5.135)$$

This has eigenfunctions  $e^{ikx}$  with eigenvalues  $k$ . The spectrum is therefore the entire real line. The local eigenvalue density of states is  $1/2\pi$ . The resolvent is therefore

$$(-i\partial_x - \lambda)_{x,\xi}^{-1} = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{ik(x-\xi)} \frac{1}{k - \lambda} dk. \quad (5.136)$$

To evaluate this, first consider the Fourier transforms of

$$\begin{aligned} F_1(x) &= \theta(x)e^{-\kappa x}, \\ F_2(x) &= -\theta(-x)e^{\kappa x}, \end{aligned} \quad (5.137)$$

where  $\kappa$  is a positive real number.

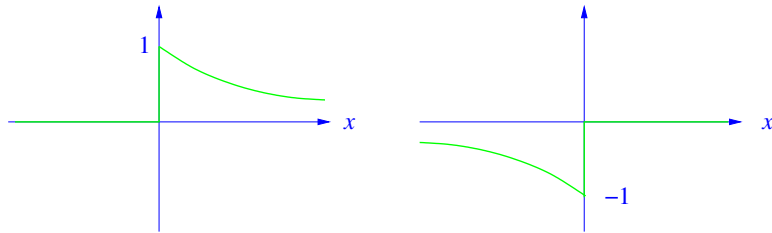


Figure 5.11: The functions  $F_1(x) = \theta(x)e^{-\kappa x}$  and  $F_2(x) = -\theta(-x)e^{\kappa x}$ .

We have

$$\int_{-\infty}^{\infty} \left\{ \theta(x) e^{-\kappa x} \right\} e^{-ikx} dx = \frac{1}{i} \frac{1}{k - i\kappa}, \quad (5.138)$$

$$\int_{-\infty}^{\infty} \left\{ -\theta(-x) e^{\kappa x} \right\} e^{-ikx} dx = \frac{1}{i} \frac{1}{k + i\kappa}. \quad (5.139)$$

Inverting the transforms gives

$$\begin{aligned} \theta(x) e^{-\kappa x} &= \frac{1}{2\pi i} \int_{-\infty}^{\infty} \frac{1}{k - i\kappa} e^{ikx} dk, \\ -\theta(-x) e^{\kappa x} &= \frac{1}{2\pi i} \int_{-\infty}^{\infty} \frac{1}{k + i\kappa} e^{ikx} dk. \end{aligned} \quad (5.140)$$

These are important formulæ in their own right, and you should take care to understand them. Now we apply them to evaluating the integral defining  $R_\lambda$ .

If we write  $\lambda = \mu + i\nu$ , we find

$$\frac{1}{2\pi} \int_{-\infty}^{\infty} e^{ik(x-\xi)} \frac{1}{k - \lambda} dk = \begin{cases} i\theta(x - \xi) e^{i\mu(x-\xi)} e^{-\nu(x-\xi)}, & \nu > 0, \\ -i\theta(\xi - x) e^{i\mu(x-\xi)} e^{-\nu(x-\xi)}, & \nu < 0, \end{cases} \quad (5.141)$$

In each case, the resolvent is  $\propto e^{i\lambda x}$  away from  $\xi$ , and has jump of  $+i$  at  $x = \xi$  so as to produce the delta function. It decays either to the right or to the left, depending on the sign of  $\nu$ . The Heaviside factor ensures that it is multiplied by zero on the exponentially growing side of  $e^{-\nu x}$ , so as to satisfy the requirement of square integrability.

Taking the trace of this resolvent is a little problematic. We are to set  $x = \xi$  and integrate — but what value do we associate with  $\theta(0)$ ? Remembering that Fourier transforms always give to the mean of the two values at a jump discontinuity, it seems reasonable to set  $\theta(0) = \frac{1}{2}$ . With this definition, we have

$$\text{Tr } R_\lambda = \begin{cases} \frac{i}{2} L, & \text{Im } \lambda > 0, \\ -\frac{i}{2} L, & \text{Im } \lambda < 0. \end{cases} \quad (5.142)$$

Our choice is therefore compatible with  $\text{Tr } R_{\lambda+i\varepsilon} = \pi\rho = L/2\pi$ . We have been lucky. The ambiguous expression  $\theta(0)$  is not always safely evaluated as  $1/2$ .

## 5.6 Locality and the Gelfand-Dikii equation

The answers to many quantum physics problems can be expressed either as sums over wavefunctions or as expressions involving Green functions. One of the advantages of writing the answer in terms of Green functions is that these typically depend only on the local properties of the differential operator whose inverse they are. This locality is in contrast to the individual wavefunctions and their eigenvalues, both of which are sensitive to the distant boundaries. Since physics is usually local, it follows that the Green function provides a more efficient route to the answer.

By the Green function being *local* we mean that its value for  $x, \xi$  near some point can be computed in terms of the coefficients in the differential operator evaluated near this point. To illustrate this claim, consider the Green function  $G(x, \xi)$  for the Schrödinger operator  $-\partial_x^2 + q(x) + \lambda$  on the entire real line. We will show that there is a not exactly obvious (but easy to obtain once you know the trick) local gradient expansion for the diagonal elements  $D(x) \equiv G(x, x)$ . These elements are often all that is needed in physics. We begin by recalling that we can write

$$G(x, \xi) \propto u(x)v(\xi)$$

where  $u(x), v(x)$  are solutions of  $(-\partial_x^2 + q(x) + \lambda)y = 0$  satisfying suitable boundary conditions to the right and left respectively. We set  $D(x) = G(x, x)$  and differentiate three times with respect to  $x$ . We find

$$\begin{aligned} \partial_x^3 D(x) &= u^{(3)}v + 3u''v' + 3u'v'' + uv^{(3)} \\ &= (\partial_x(q + \lambda)u)v + 3(q + \lambda)\partial_x(uv) + (\partial_x(q + \lambda)v)u. \end{aligned}$$

Here, in passing from the first to second line, we have used the differential equation obeyed by  $u$  and  $v$ . We can re-express the second line as

$$(q\partial_x + \partial_x q - \frac{1}{2}\partial_x^3)D(x) = -2\lambda\partial_x D(x). \quad (5.143)$$

This relation is known as the *Gelfand-Dikii equation*. Using it we can find an expansion for the diagonal element  $D(x)$  in terms of  $q$  and its derivatives. We begin by observing that for  $q(x) \equiv 0$  we know that  $D(x) = 1/(2\sqrt{\lambda})$ . We therefore conjecture that we can expand

$$D(x) = \frac{1}{2\sqrt{\lambda}} \left( 1 - \frac{b_1(x)}{2\lambda} + \frac{b_2(x)}{(2\lambda)^2} + \cdots + (-1)^n \frac{b_n(x)}{(2\lambda)^n} + \cdots \right).$$

If we insert this expansion into (5.143) we see that we get the recurrence relation

$$(q\partial_x + \partial_x q - \frac{1}{2}\partial_x^3)b_n = \partial_x b_{n+1}. \quad (5.144)$$

We can therefore find  $b_{n+1}$  from  $b_n$  by differentiation followed by a single integration. Remarkably,  $\partial_x b_{n+1}$  is always the exact derivative of a polynomial in  $q$  and its derivatives. Further, the integration constants must be zero so that we recover the  $q \equiv 0$  result. If we carry out this process, we find

$$\begin{aligned} b_1(x) &= q(x), \\ b_2(x) &= \frac{3q(x)^2}{2} - \frac{q''(x)}{2}, \\ b_3(x) &= \frac{5q(x)^3}{2} - \frac{5q'(x)^2}{4} - \frac{5q(x)q''(x)}{2} + \frac{q^{(4)}(x)}{4}, \\ b_4(x) &= \frac{35q(x)^4}{8} - \frac{35q(x)q'(x)^2}{4} - \frac{35q(x)^2q''(x)}{4} + \frac{21q''(x)^2}{8} \\ &\quad + \frac{7q'(x)q^{(3)}(x)}{2} + \frac{7q(x)q^{(4)}(x)}{4} - \frac{q^{(6)}(x)}{8}, \end{aligned} \quad (5.145)$$

and so on. (Note how the terms in the expansion are graded: Each  $b_n$  is homogeneous in powers of  $q$  and its derivatives, provided we count two  $x$  derivatives as being worth one  $q(x)$ .) Keeping a few terms in this series expansion can provide an effective approximation for  $G(x, x)$ , but, in general, the series is not convergent, being only an *asymptotic expansion* for  $D(x)$ .

A similar strategy produces expansions for the diagonal element of the Green function of other one-dimensional differential operators. Such gradient expansions also exist in higher dimensions but the higher-dimensional *Seeley-coefficient* functions are not as easy to compute. Gradient expansions for the off-diagonal elements also exist, but, again, they are harder to obtain.

## 5.7 Further exercises and problems

Here are some further exercises that are intended to illustrate the material of this chapter:

*Exercise 5.1: Fredholm Alternative.* A heavy elastic bar with uniform mass  $m$  per unit length lies almost horizontally. It is supported by a distribution of upward forces  $F(x)$ .

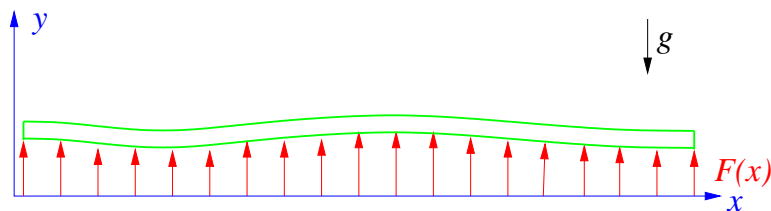


Figure 5.12: Elastic bar

The shape of the bar,  $y(x)$ , can be found by minimizing the energy

$$U[y] = \int_0^L \left\{ \frac{1}{2} \kappa (y'')^2 - (F(x) - mg)y \right\} dx.$$

- Show that this minimization leads to the equation

$$\widehat{L}y \equiv \kappa \frac{d^4 y}{dx^4} = F(x) - mg, \quad y'' = y''' = 0 \quad \text{at } x = 0, L.$$

- Show that the boundary conditions are such that the operator  $\widehat{L}$  is self-adjoint with respect to an inner product with weight function 1.
- Find the zero modes which span the null space of  $\widehat{L}$ .
- If there are  $n$  linearly independent zero modes, then the codimension of the range of  $\widehat{L}$  is also  $n$ . Using your explicit solutions from the previous part, find the conditions that must be obeyed by  $F(x)$  for a solution of  $\widehat{L}y = F - mg$  to exist. What is the physical meaning of these conditions?
- The solution to the equation and boundary conditions is not unique. Is this non-uniqueness physically reasonable? Explain.

*Exercise 5.2: Flexible rod again.* A flexible rod is supported near its ends by means of knife edges that constrain its position, but not its slope or curvature. It is acted on by a force  $F(x)$ .

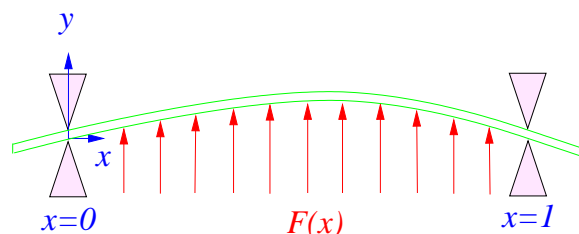
The deflection of the rod is found by solving the the boundary value problem

$$\frac{d^4 y}{dx^4} = F(x), \quad y(0) = y(1) = 0, \quad y''(0) = y''(1) = 0.$$

We wish to find the Green function  $G(x, \xi)$  that facilitates the solution of this problem.

- If the differential operator and domain (boundary conditions) above is denoted by  $L$ , what is the operator and domain for  $L^\dagger$ ? Is the problem self-adjoint?



Figure 5.13: *Simply supported rod.*

- b) Are there any zero-modes? Does  $F$  have to satisfy any conditions for the solution to exist?
- c) Write down the conditions, if any, obeyed by  $G(x, \xi)$  and its derivatives  $\partial_x G(x, \xi)$ ,  $\partial_{xx}^2 G(x, \xi)$ ,  $\partial_{xxx}^3 G(x, \xi)$  at  $x = 0$ ,  $x = \xi$ , and  $x = 1$ .
- d) Using the conditions above, find  $G(x, \xi)$ . (This requires some boring algebra — but if you start from the “jump condition” and work down, it can be completed in under a page)
- e) Is your Green function symmetric ( $G(x, \xi) = G(\xi, x)$ )? Is this in accord with the self-adjointness or not of the problem? (You can use this property as a check of your algebra.)
- f) Write down the integral giving the general solution of the boundary value problem. Assume, if necessary, that  $F(x)$  is in the range of the differential operator. Differentiate your answer and see if it does indeed satisfy the differential equation and boundary conditions.

*Exercise 5.3: Hot ring.* The equation governing the steady state heat flow on thin ring of unit circumference is

$$-y'' = f, \quad 0 < x < 1, \quad y(0) = y(1), \quad y'(0) = y'(1).$$

- a) This problem has a zero mode. Find the zero mode and the consequent condition on  $f(x)$  for a solution to exist.
- b) Verify that a suitable modified Green function for the problem is

$$g(x, \xi) = \frac{1}{2}(x - \xi)^2 - \frac{1}{2}|x - \xi|.$$

You will need to verify that  $g(x, \xi)$  satisfies both the differential equation and the boundary conditions.

*Exercise 5.4:* By using the observation that the left hand side is  $2\pi$  times the eigenfunction expansion of a modified Green function  $G(x, 0)$  for  $L = -\partial_x^2$  on a circle of unit radius, show that

$$\sum_{n=-\infty}^{\infty} \frac{e^{inx}}{n^2} = \frac{1}{2}(x - \pi)^2 - \frac{\pi^2}{6}, \quad x \in [0, 2\pi).$$

The term with  $n = 0$  is to be omitted from the sum.

*Exercise 5.5:* Seek a solution to the equation

$$-\frac{d^2y}{dx^2} = f(x), \quad x \in [0, 1]$$

with inhomogeneous boundary conditions  $y'(0) = F_0$ ,  $y'(1) = F_1$ . Observe that the corresponding homogeneous boundary condition problem has a zero mode. Therefore the solution, if one exists, cannot be unique.

- a) Show that there can be no solution to the differential equation and inhomogeneous boundary condition unless  $f(x)$  satisfies the condition

$$\int_0^1 f(x) dx = F_0 - F_1. \quad (\star)$$

- b) Let  $G(x, \xi)$  denote the modified Green function (5.57)

$$G(x, \xi) = \begin{cases} \frac{1}{3} - \xi + \frac{x^2 + \xi^2}{2}, & 0 < x < \xi \\ \frac{1}{3} - x + \frac{x^2 + \xi^2}{2}, & \xi < x < 1, \end{cases}$$

Use the Lagrange-identity method for inhomogeneous boundary conditions to deduce that if a solution exists then it necessarily obeys

$$y(x) = \int_0^1 y(\xi) d\xi + \int_0^1 G(\xi, x) f(\xi) d\xi + G(1, x)F_1 - G(0, x)F_0.$$

- c) By differentiating with respect to  $x$ , show that

$$y_{\text{tentative}}(x) = \int_0^1 G(\xi, x) f(\xi) d\xi + G(1, x)F_1 - G(0, x)F_0 + C,$$

where  $C$  is an arbitrary constant, obeys the boundary conditions.

- d) By differentiating a second time with respect to  $x$ , show that  $y_{\text{tentative}}(x)$  is a solution of the differential equation if, and only if, the condition  $\star$  is satisfied.

*Exercise 5.6: Lattice Green Functions.* The  $k \times k$  matrices

$$\mathbf{T}_1 = \begin{pmatrix} 2 & -1 & 0 & 0 & 0 & \dots & 0 \\ -1 & 2 & -1 & 0 & 0 & \dots & 0 \\ 0 & -1 & 2 & -1 & 0 & \dots & 0 \\ \vdots & \vdots & \ddots & \ddots & \ddots & \vdots & \vdots \\ 0 & \dots & 0 & -1 & 2 & -1 & 0 \\ 0 & \dots & 0 & 0 & -1 & 2 & -1 \\ 0 & \dots & 0 & 0 & 0 & -1 & 2 \end{pmatrix}, \quad \mathbf{T}_2 = \begin{pmatrix} 2 & -1 & 0 & 0 & 0 & \dots & 0 \\ -1 & 2 & -1 & 0 & 0 & \dots & 0 \\ 0 & -1 & 2 & -1 & 0 & \dots & 0 \\ \vdots & \vdots & \ddots & \ddots & \ddots & \vdots & \vdots \\ 0 & \dots & 0 & -1 & 2 & -1 & 0 \\ 0 & \dots & 0 & 0 & -1 & 2 & -1 \\ 0 & \dots & 0 & 0 & 0 & -1 & 1 \end{pmatrix}$$

represent two discrete lattice approximations to  $-\partial_x^2$  on a finite interval.

- What are the boundary conditions defining the domains of the corresponding continuum differential operators? [They are either Dirichlet ( $y = 0$ ) or Neumann ( $y' = 0$ ) boundary conditions.] Make sure you explain your reasoning.
- Verify that

$$[\mathbf{T}_1^{-1}]_{ij} = \min(i, j) - \frac{ij}{k+1},$$

$$[\mathbf{T}_2^{-1}]_{ij} = \min(i, j).$$

- Find the continuum Green functions for the boundary value problems approximated by the matrix operators. Compare each of the matrix inverses with its corresponding continuum Green function. Are they similar?

*Exercise 5.7: Eigenfunction expansion* The resolvent (Green function)  $R_\lambda(x, \xi) = (L - \lambda)_{x\xi}^{-1}$  can be expanded as

$$(L - \lambda)_{x\xi}^{-1} = \sum_{\lambda_n} \frac{\varphi_n(x)\varphi_n(\xi)}{\lambda_n - \lambda},$$

where  $\varphi_n(x)$  is the normalized eigenfunction corresponding to the eigenvalue  $\lambda_n$ . The resolvent therefore has a *pole* whenever  $\lambda$  approaches  $\lambda_n$ . Consider the case

$$R_{\omega^2}(x, \xi) = \left( -\frac{d^2}{dx^2} - \omega^2 \right)_{x\xi}^{-1},$$

with boundary conditions  $y(0) = y(L) = 0$ .

- Show that

$$\begin{aligned} R_{\omega^2}(x, \xi) &= \frac{1}{\omega \sin \omega L} \sin \omega x \sin \omega(L - \xi), \quad x < \xi, \\ &= \frac{1}{\omega \sin \omega L} \sin \omega(L - x) \sin \omega \xi, \quad \xi < x \end{aligned}$$

- b) Confirm that  $R_{\omega^2}$  becomes singular at exactly those values of  $\omega^2$  corresponding to eigenvalues  $\omega_n^2$  of  $-\frac{d^2}{dx^2}$ .
- c) Find the associated eigenfunctions  $\varphi_n(x)$  and, by taking the limit of  $R_{\omega^2}$  as  $\omega^2 \rightarrow \omega_n^2$ , confirm that the *residue* of the pole (the coefficient of  $1/(\omega_n^2 - \omega^2)$ ) is precisely the product of the *normalized* eigenfunctions  $\varphi_n(x)\varphi_n(\xi)$ .

*Exercise 5.8:* In this exercise we will investigate the self adjointness of the operator  $T = -i\partial/\partial x$  on the interval  $[a, b]$  by using the resolvent operator  $R_\lambda = (T - \lambda I)^{-1}$ .

- a) The integral kernel  $R_\lambda(x, \xi)$  is a Green function obeying

$$\left(-i\frac{\partial}{\partial x} - \lambda\right) R_\lambda(x, \xi) = \delta(x - \xi).$$

Use standard methods to show that

$$R_\lambda(x, \xi) = \frac{1}{2} \left( K_\lambda + i \operatorname{sgn}(x - \xi) \right) e^{i\lambda(x - \xi)},$$

where  $K_\lambda$  is a number that depends on the boundary conditions imposed at the endpoints  $a, b$ , of the interval.

- b) If  $T$  is to be self-adjoint then the Green function must be Hermitian, *i.e.*  $R_\lambda(x, \xi) = [R_\lambda(\xi, x)]^*$ . Find the condition on  $K_\lambda$  for this to be true, and show that it implies that

$$\frac{R_\lambda(b, \xi)}{R_\lambda(a, \xi)} = e^{i\theta_\lambda},$$

where  $\theta_\lambda$  is some real angle. Deduce that the range of  $R_\lambda$  is the set of functions

$$\mathcal{D}_\lambda = \{y(x) : y(b) = e^{i\theta_\lambda} y(a)\}.$$

Now the range of  $R_\lambda$  is the domain of  $(T - \lambda I)$ , which should be same as the domain of  $T$  and therefore not depend on  $\lambda$ . We therefore require that  $\theta_\lambda$  not depend on  $\lambda$ . Deduce that  $T$  will be self-adjoint only for boundary conditions  $y(b) = e^{i\theta} y(a)$  — *i.e.* for twisted periodic boundary conditions.

- c) Show that with the twisted periodic boundary conditions of part b), we have

$$K_\lambda = -\cot\left(\frac{\lambda(b - a) - \theta}{2}\right).$$

From this, show that  $R_\lambda(x, \xi)$  has simple poles at  $\lambda = \lambda_n$ , where  $\lambda_n$  are the eigenvalues of  $T$ .

- d) Compute the residue of the pole of  $R_\lambda(x, \xi)$  at the eigenvalue  $\lambda_n$ , and confirm that it is a product of the corresponding normalized eigenfunctions.

*Problem 5.9:* Consider the one-dimensional Dirac Hamiltonian

$$\begin{aligned}\widehat{H} &= \begin{pmatrix} -i\partial_x & m_1 - im_2 \\ m_1 + im_2 & +i\partial_x \end{pmatrix}, \\ &= -i\widehat{\sigma}_3\partial_x + m_1(x)\widehat{\sigma}_1 + m_2(x)\widehat{\sigma}_2.\end{aligned}$$

Here  $m_1(x)$ ,  $m_2(x)$  are real functions, and the  $\widehat{\sigma}_i$  are the Pauli matrices.  $\widehat{H}$  acts on a two-component “spinor”

$$\Psi(x) = \begin{pmatrix} \psi_1(x) \\ \psi_2(x) \end{pmatrix}.$$

Impose self-adjoint boundary conditions

$$\frac{\psi_1(a)}{\psi_2(a)} = \exp\{i\theta_a\}, \quad \frac{\psi_1(b)}{\psi_2(b)} = \exp\{i\theta_b\}$$

at the ends of the interval  $[a, b]$ . Let  $\Psi_L(x)$  be a solution of  $\widehat{H}\Psi = \lambda\Psi$  obeying the boundary condition at  $x = a$ , and  $\Psi_R(x)$  be a solution obeying the boundary condition at  $x = b$ . Define the “Wronskian” of these solutions to be

$$W(\Psi_L, \Psi_R) = \Psi_L^\dagger \widehat{\sigma}_3 \Psi_R.$$

- a) Show that, for real  $\lambda$  and the given boundary conditions, the Wronskian  $W(\Psi_L, \Psi_R)$  is independent of position. Show also that  $W(\Psi_L, \Psi_L) = W(\Psi_R, \Psi_R) = 0$ .
- b) Show that the matrix-valued Green function  $\widehat{G}(x, \xi)$  obeying

$$(\widehat{H} - \lambda I)\widehat{G}(x, \xi) = I\delta(x - \xi),$$

and the given boundary conditions has entries

$$G_{\alpha\beta}(x, \xi) = \begin{cases} -\frac{i}{W^*}\psi_{L,\alpha}(x)\psi_{R,\beta}^*(\xi), & x < \xi, \\ +\frac{i}{W}\psi_{R,\alpha}(x)\psi_{L,\beta}^*(\xi), & x > \xi. \end{cases}$$

Observe that  $G_{\alpha\beta}(x, \xi) = G_{\beta\alpha}^*(\xi, x)$ , as befits the inverse of a self-adjoint operator.

- c) The Green function is discontinuous at  $x = \xi$ , but we can define a “position-diagonal” part by the taking the average

$$G_{\alpha\beta}(x) \stackrel{\text{def}}{=} \frac{1}{2} \left( \frac{i}{W} \psi_{R,\alpha}(x) \psi_{L,\beta}^*(x) - \frac{i}{W^*} \psi_{L,\alpha}(x) \psi_{R,\beta}^*(x) \right).$$

Show that if we define the matrix  $\hat{g}(x)$  by setting  $\hat{g}(x) = \hat{G}(x)\hat{\sigma}_3$ , then  $\text{tr} \hat{g}(x) = 0$  and  $\hat{g}^2(x) = -\frac{1}{4}I$ . Show further that

$$i\partial_x \hat{g} = [\hat{g}, \hat{K}], \quad (\star)$$

where  $\hat{K}(x) = \hat{\sigma}_3 (\lambda I - m_1(x)\hat{\sigma}_1 - m_2(x)\hat{\sigma}_2)$ .

The equation  $(\star)$  obtained in part (c) is the analogue of the Gelfand-Dikii equation for the Dirac Hamiltonian. It has applications in the theory of superconductivity, where  $(\star)$  is known as the *Eilenberger equation*.