Green's Functions

Green's Function of the Sturm-Liouville Equation

Consider the problem of finding a function $u = u(x)$, $x \in [a, b]$, satisfying canonical boundary conditions at the points a and b, and the equation

$$Lu(x) = f(x) \ , \tag{1}$$

where

$$L = \frac{1}{w(x)} \left[\frac{d}{dx} p(x) \frac{d}{dx} - q(x) \right] \tag{2}$$

is the Sturm-Liouville operator. As we have found previously, the solution of this problem, if exists, can be found in the form of the Fourier series in terms of the eigenfunctions of the operator L:

$$u(x) = \sum_m u_m e_m(x) \ , \tag{3}$$

$$Le_m(x) = \lambda_m e_m(x) \ , \tag{4}$$

where each Fourier coefficient u_m satisfies the equation

$$\lambda_m u_m = \langle e_m | f \rangle \equiv \int_a^b e_m^*(x) f(x) w(x) \, dx \ . \tag{5}$$

The solution for (5) exists in the following two cases. (i) When $\lambda_m \neq 0 \ \forall \, m$. (ii) When there exist zero λ's, but $\langle e_m | f \rangle = 0 \ \ \forall \, \lambda_m = 0$.

From now on we will be dealing only with the case (i), when there is no restriction on the form of $f(x)$. Eq. (5) implies

$$u_m = \lambda_m^{-1} \int_a^b e_m^*(x) f(x) w(x) \, dx \ . \tag{6}$$

If we plug (5) into (3) and interchange the orders of summation and integration, we arrive at an interesting observation. The solution comes in a simple form of the integral

$$u(x) = \int_a^b G(x, x_0) w(x_0) f(x_0) \, dx_0 \ , \tag{7}$$

where $G(x, x_0)$ is a certain f-independent function:

$$G(x, x_0) = \sum_m \lambda_m^{-1} \, e_m(x) \, e_m^*(x_0) \ . \tag{8}$$

This function is called *Green's function.*

Once we realize that such a function exists, we would like to find it explicitly—without summing up the series (8). The idea is to directly formulate the problem for $G(x, x_0)$, by excluding the arbitrary function $f(x)$. First, from (8) we note that as a function of variable x, the Green's function satisfies the same canonical boundary conditions as the functions $u(x)$ and all $e_m(x)$'s. [Because the canonical boundary conditions feature the vector property—they are satisfied by any linear combination of functions satisfying them individually.] Given the boundary conditions, we want to find a differential equation for $G(x, x_0)$. To this end we act with the operator L on both sides of (7) and interchange the orders of L and integration. With (1) taken into account, we get

$$\int_a^b \tilde{L}\, G(x, x_0) \tilde{f}(x_0)\, dx_0 \;=\; \tilde{f}(x) \;, \tag{9}$$

where

$$\tilde{L} \;=\; \frac{d}{dx}\, p(x) \frac{d}{dx} - q(x) \tag{10}$$

and

$$\tilde{f}(x) \;=\; f(x)\, w(x) \;. \tag{11}$$

Now we see that actually it was illegal to interchange the orders: According to (9), the function $\tilde{L}\, G(x, x_0)$ is nothing else than the δ-function $\delta(x - x_0)$, which is a *generalized* rather than a regular function. Here we do not see a special reason for working with generalized functions, and make one step back. The δ-function arises when one differentiates (inside an integral) a stepwise function. Hence, we understand—or at least suspect—that the function $G(x, x_0)$ has a discontinuous partial derivative at $x = x_0$. This means that we need to be more careful with the differentiation.—Prior to interchange the orders with respect to the *second* differentiation, we have to split the integral into two parts:

$$\int_a^b p(x) G_x(x, x_0) \tilde{f}(x_0) dx_0 \;=$$
$$= \int_a^{x-0} p(x) G_x(x, x_0) \tilde{f}(x_0) dx_0 + \int_{x+0}^b p(x) G_x(x, x_0) \tilde{f}(x_0) dx_0 \;. \tag{12}$$

Now each function is differentiable, since the point $x = x_0$ is excluded. We thus have

$$\frac{d}{dx} \int_a^b p(x) G_x(x, x_0) \tilde{f}(x_0) dx_0 \;=$$

$$= \frac{d}{dx}\int_a^{x-0} p(x)G_x(x,x_0)\tilde f(x_0)dx_0 + \frac{d}{dx}\int_{x+0}^{b} p(x)G_x(x,x_0)\tilde f(x_0)dx_0 =$$
$$= p(x)G_x(x,x-0)\tilde f(x) \,+\, \int_a^{x-0}\frac{d}{dx}\,p(x)G_x(x,x_0)\tilde f(x_0)dx_0 -$$
$$-p(x)G_x(x,x+0)\tilde f(x) \,+\, \int_{x+0}^{b}\frac{d}{dx}\,p(x)G_x(x,x_0)\tilde f(x_0)dx_0 \;.$$

Then, the correct version of (9) reads

$$p(x)\left[G_x(x,x-0) - G_x(x,x+0)\right]\tilde f(x) \,+$$
$$+\int_a^{x-0}\tilde L G(x,x_0)\tilde f(x_0)dx_0 \,+\, \int_{x+0}^{b}\tilde L G(x,x_0)\tilde f(x_0)dx_0 \;=\; \tilde f(x)\;. \tag{13}$$

Clearly, Eq. (13) is satisfied if

$$\tilde L G(x,x_0) \;=\; 0 \qquad\qquad (x \neq x_0) \tag{14}$$

and

$$p(x)\left[G_x(x,x-0) - G_x(x,x+0)\right] \;=\; 1\;. \tag{15}$$

Hence, to find $G(x,x_0)$ we need to solve Eq. (14) with the given canonical boundary conditions at the points a and b, and with the additional condition (15) at the point $x = x_0$, where the partial derivative experiences a jump. The function itself does not have any jump at $x = x_0$. This leads to one more condition:

$$G(x,x-0) \;=\; G(x,x+0)\;. \tag{16}$$

The problem (14)-(16) with the canonical boundary conditions is solved as follows. We look for the solution of the form

$$G(x,x_0) \;=\; \begin{cases} A(x_0)\,U(x)\;, & x < x_0\;,\\ B(x_0)\,V(x)\;, & x > x_0\;,\end{cases} \tag{17}$$

where

$$\tilde L U(x) = 0\;, \qquad \tilde L V(x) = 0 \tag{18}$$

and $U(x)$ satisfies the boundary condition at the point a, while $V(x)$ satisfies the boundary condition at the point b. With this form, Eq. (14) and the boundary conditions at the points a and b are satisfied, and we have to find the functions $A(x_0)$ and $B(x_0)$ from the conditions (15)-(16):

$$p(x)\left[B(x)\,V'(x) - A(x)\,U'(x)\right] \;=\; 1\;, \tag{19}$$

$$A(x)\,U(x) \;=\; B(x)\,V(x)\;. \tag{20}$$

Solving the system (19)-(20), we find

$$A(x) \;=\; C(x)\,V(x)\;, \qquad\qquad B(x) \;=\; C(x)\,U(x)\;, \tag{21}$$

where

$$C(x) \;=\; \frac{1}{p(x)\,[U(x)\,V'(x) - V(x)\,U'(x)]}\;. \tag{22}$$

Actually, C is just a constant. To make sure this is the case, we calculate $[1/C(x)]'$ with Eq. (18) taken into account:

$$\frac{d}{dx}\,p\frac{d}{dx}\,U \;=\; qU\;, \qquad \frac{d}{dx}\,p\frac{d}{dx}\,V \;=\; qV\;. \tag{23}$$

We have

$$[1/C(x)]' \;=\; \frac{d}{dx}\,p\,[U\,V' - V\,U'] \;=$$
$$=\; p\,U'\,V' \,+\, U\frac{d}{dx}\,p\,\frac{d}{dx}\,V \,-\, p\,V'\,U' \,-\, V\frac{d}{dx}\,p\,\frac{d}{dx}\,U \;=\; qUV - qVU \;=\; 0\,.$$

The final answer reads

$$G(x,x_0) \;=\; \begin{cases} C\,V(x_0)\,U(x)\;, & x < x_0\;, \\ C\,U(x_0)\,V(x)\;, & x > x_0\;. \end{cases} \tag{24}$$

The meaning of the constant C is quite transparent. The canonical boundary conditions fix the form of the functions U and V only up to some normalization factors. The constant C eliminates this arbitrariness.

Problem 33. Consider the problem

$$u''(x) - \gamma^2 u(x) = f(x)\;, \qquad x \in [0,1]\;, \tag{25}$$

$$u(0) = 0\;, \qquad u'(1) = 0\;, \tag{26}$$

$f(x)$ is a given function, γ is a real—positive, without loss of generality—number.

(a) Construct the Green's function for this problem.

(b) With the Green's function constructed, find the solution for $f(x) = x$. Make sure that your solution is correct by explicitly checking that it satisfies (25)-(26).

Green's Function of a Time-Dependent Linear PDE

Consider a one-dimensional heat (or Schrödinger, if $\gamma = -i$) equation

$$\gamma u_t = u_{xx} \;, \tag{27}$$

where $u = u(x,t)$, $x \in (-\infty, \infty)$. We want to find $u(x,t)$ for a given initial condition

$$u(x, t=0) = q(x) \;. \tag{28}$$

Suppose for a while, that $x \in [-a/2, a/2]$ and at $x = \pm a/2$ we have some canonical boundary conditions. Later on we will take the limit of $a \to \infty$ and the particular form of boundary conditions will not be important. The problem has a form of the differential equation in a Hilbert space:

$$(d/dt)|u(t)\rangle = L|u(t)\rangle \;, \tag{29}$$

where $L = \nabla^2$ is a self-adjoint operator. We have already considered this problem and have demonstrated that the solution of (29) can be written as a Fourier series over the orthonormal basis of the eigenvectors of the operator L:

$$|u(t)\rangle \;=\; \sum_m u_m \mathrm{e}^{\lambda_m t/\gamma}\, |e_m\rangle \;, \tag{30}$$

$$L|e_m\rangle = \lambda_m |e_m\rangle \;, \tag{31}$$

$$u_m = \langle e_m | q \rangle \;. \tag{32}$$

Translating into the language of functions, where the inner product is understood as an integral, we see that

$$u(x,t) = \int G(x, x_0, t)\, q(x_0)\, dx_0 \;, \tag{33}$$

where

$$G(x, x_0, t) \;=\; \sum_m \mathrm{e}^{\lambda_m t/\gamma}\, e_m(x) e_m^*(x_0) \;. \tag{34}$$

The function G is called Green's function. Green's function allows one to obtain $u(x,t)$ from $u(x,0)$ by a simple procedure of doing an integral.

A note is in order here. When obtaining (33) we interchanged the orders of integration and summation which might be not legitimate within the set of ordinary functions. This means that in certain cases G should be understood as a *generalized* function, which is even better from the practical viewpoint.—The integrals with the generalized functions are easily done!

How can we find G explicitly? And why do we expect G to exist in the limit of $a \to \infty$? We start from the second question. Physically we understand that if a is large enough and our $u(x,t)$ is well-behaved in the sense that it is practically zero already at $|x| \ll a$, then the evolution of u should be independent of a, which implies that if $a \to \infty$, then G approaches some a-independent limit, corresponding to the case $x \in (-\infty, \infty)$.

To find G, we act with the operator $\hat{O} = \gamma\partial/\partial t - \partial^2/\partial x^2$ on both sides of Eq. (33) to obtain

$$\int \hat{O}G(x,x_0,t)\, q(x_0)\, dx_0 = 0 \; . \tag{35}$$

Since (35) is supposed to be valid for *any* function $q(x_0)$, we conclude that

$$\hat{O}G(x,x_0,t) = 0 \; . \tag{36}$$

Considering Eq. (33) in the limit of $t \to 0$ we see that for *any* function $q(x)$

$$\lim_{t\to 0} \int G(x,x_0,t)\, q(x_0)\, dx_0 \; = \; q(x) \; . \tag{37}$$

From Eq. (37) it is seen that the function $G(x,x_0,t)$ becomes singular—infinitely sharp, but infinitely narrow peak—in the limit of $t \to 0$. Actually, Eq. (37) is nothing else than the definition of the δ-function, so that one can write

$$G(x,x_0,0) = \delta(x - x_0) \; . \tag{38}$$

In this section, however, we are not going to work with the generalized functions and for the present purposes the limiting relation (37) is quite sufficient.

Now we take into account that in the limit $a \to \infty$ the problem becomes translation invariant: If $u(x,t)$ is a solution of our problem, then the shifted function, $u(x - x_*, t)$, where x_* is a constant, is also a solution that corresponds to a shifted by x_* initial condition, $q(x) \to g(x - x_*)$. To be consistent with translational invariance, the form of the Green's function should be the following:

$$G(x,x_0,t) \equiv G(x - x_0, t). \tag{39}$$

That is instead of three independent variables we have just two. In view of Eq. (39), the relation (37) can be re-written as

$$\lim_{t\to 0} \int G(\tilde{x},t)\, q(x-\tilde{x})\, d\tilde{x} \; = \; q(x) \; , \qquad\qquad \forall\, q(x) \; , \tag{40}$$

and then, introducing $\tilde{q}(\tilde{x}) = q(x - \tilde{x})$ and ultimately replacing $\tilde{x}$ with x:

$$\lim_{t \to 0} \int G(x,t)\, \tilde{q}(x)\, dx \;=\; \tilde{q}(0)\;, \qquad\qquad \forall\, \tilde{q}(x)\;. \tag{41}$$

Hence, to obtain the function $G(x,t)$ we need to find the solution of the equation

$$\gamma G_t = G_{xx} \tag{42}$$

that satisfies the initial condition (41). Below we will do it by revealing and utilizing the *self-similarity* of $G(x,t)$.

A physicist's approach to self-similarity of $G(x,t)$

Looking at the equations (42) and (41), a physicist immediately notices that while the function $G(x,t)$ depends on two dimensional variables, x and t, there is *only one* dimensional constant in the problem—the parameter γ which dimensionality is time over distance squared. This means that the only possible dimensionless combination of x and t is

$$\xi = \gamma x^2/t\;. \tag{43}$$

Then, as it is clearly seen from (41), the dimensionality of G is the inverse distance. From this analysis of dimensions we conclude that the Green's function should have the form

$$G(x,t) \;=\; \sqrt{\frac{\gamma}{t}}\, g(\gamma x^2/t)\;, \tag{44}$$

where g is a certain dimensionless function. It is easy to see that this form is consistent with (41). Moreover, plugging (44) into (41), changing the variable of integration from x to the dimensionless variable $y = \sqrt{\xi}$, and choosing $\tilde{q} \equiv 1$, we find the normalization condition

$$\int g(y^2)\, dy = 1\;. \tag{45}$$

Eq. (44) means that the function $G(x,t)$ is *self-similar* in the sense that at different time moments the spatial profile of G remains the same up to re-scaling the coordinate units and the units of G.

Eq. (44) radically simplifies the problem of obtaining G by reducing PDE (42) to an ordinary differential equation. Prior to resorting to this equation, we introduce an alternative, purely formal, way of arriving at Eq. (44).

Scale invariance and self-similarity of G

Let $u(x,t)$ be a solution of the equation (27). Consider the *scaling transformation*

$$u(x,t) \to \tilde{u}(x,t) = \lambda u(\lambda^{\alpha} x, \lambda^{\beta} t) \ , \tag{46}$$

where λ, α, and β are real numbers. By a direct check we make sure that

$$\gamma \tilde{u}_t = \lambda^{\beta - 2\alpha} \, \tilde{u}_{xx} \ , \tag{47}$$

which means that with $\beta = 2\alpha$, the function $\tilde{u}(x,t)$ satisfies Eq. (27). We thus arrive at the *similarity transformation*

$$u(x,t) \to \tilde{u}(x,t) = \lambda u(\lambda^{\alpha} x, \lambda^{2\alpha} t) \ , \tag{48}$$

which, given a solution $u(x,t)$, produces a continuum of other, *similar*, solutions. The property of an equation of having similar solutions is called *scale invariance*, because it is associated with the absence of *a priory* scales for the variables.

In Eq. (48), λ and λ^{α} are actually two independent parameters. It is just a matter of convenience—see below—to write them in such a form.

In accordance with the above-established scale invariance of the equation (42), the function

$$\tilde{G}(x,t) = \lambda G(\lambda^{\alpha} x, \lambda^{2\alpha} t) \tag{49}$$

also satisfies Eq. (42). But what about the relation (41)? Introducing in Eq. (41) new variables, x' and y', by

$$x = \lambda^{\alpha} x' \ , \qquad\qquad t = \lambda^{2\alpha} t' \ , \tag{50}$$

we rewrite (41) as

$$\lim_{t' \to 0} \int G(\lambda^{\alpha} x', \lambda^{2\alpha} t') \, \tilde{q}(\lambda^{\alpha} x') \, dx' \ = \ \lambda^{-\alpha} \, \tilde{q}(0) \ , \qquad \forall \, \tilde{q}(\lambda^{\alpha} x') \ . \tag{51}$$

In terms of the function $\tilde{G}(x,t)$ this reads (below we introduce a new function, $\tilde{\tilde{q}}(x') = \tilde{q}(\lambda^{\alpha} x')$, and omit primes)

$$\lim_{t \to 0} \int \tilde{G}(x,t) \, \tilde{\tilde{q}}(x) \, dx \ = \ \lambda^{1-\alpha} \, \tilde{\tilde{q}}(0) \ , \qquad \forall \, \tilde{\tilde{q}}(x) \ . \tag{52}$$

Comparing (52) with (41), we make a remarkable observation that at $\alpha = 1$, the function $\tilde{G}$ satisfies *both* the equation (42) and the condition (41), which means that it is nothing else than the function G. Hence, we have established the *self-similarity* of the function G:

$$\lambda G(\lambda x, \lambda^2 t) \equiv G(x,t) \ . \tag{53}$$

Now we need to make sure that this formal definition of self-similarity is equivalent to what have been established previously by the physicist's argument. Without loss of generality, we may introduce the new variable $\xi = \gamma x^2/t$ instead of x and write $G(x,t) \equiv f(\xi,t)$. With the new variable, Eq. (53) reads

$$\lambda f(\xi, \lambda^2 t) \equiv f(\xi,t) \ . \tag{54}$$

Lemma. If a function $f(t)$ satisfies the relation ($\forall\, \lambda$ and a certain α)

$$\lambda f(\lambda^\alpha t) \equiv f(t) \ , \tag{55}$$

then

$$f(t) \propto t^{-1/\alpha} \ . \tag{56}$$

Proof. Differentiate (55) with respect to λ and set $\lambda = 1$. Solve the resulting first-order differential equation.

With this lemma and (54) we have

$$f(\xi,t) \propto \frac{g(\xi)}{\sqrt{t}} \ , \tag{57}$$

where $g(\xi)$ is some function of ξ. That is we have established Eq. (44) by purely mathematical tools.

Solving for $g(\xi)$

Substituting $g(\gamma x^2/t)/\sqrt{t}$ for G in (42), we get

$$\left(\frac{1}{2} + \xi\frac{\mathrm{d}}{\mathrm{d}\xi}\right)\left[4g'(\xi) + g(\xi)\right] = 0 \ . \tag{58}$$

This is a second-order ordinary differential equation. Its general solution contains two free constants to be fixed by the two conditions: (i) $g(\xi)$ should remain at least finite at $\xi \to +\infty$ and (ii) it should satisfy (45).

Eq. (58) can be solved as follows. First, one finds a solution of the supplementary first-order equation

$$\left(\frac{1}{2} + \xi\frac{\mathrm{d}}{\mathrm{d}\xi}\right)\chi(\xi) = 0 \ , \tag{59}$$

and then finds $g(\xi)$ from another first-order equation,

$$4g'(\xi) + g(\xi) = \chi(\xi) \ . \tag{60}$$

It turns out that in our case the relevant solution of Eq. (59) is just $\chi(\xi) \equiv 0$. Indeed, with $\chi \equiv 0$ we find

$$g(\xi) = A\mathrm{e}^{-\xi/4} \ , \tag{61}$$

where A is a constant. This solution does satisfy the requirement (i), and we just need to fix A by (45). This yields $A = 1/(2\sqrt{\pi})$.

The final answer for the Green's function thus is

$$G(x, x_0, t) \ = \ \frac{1}{2}\sqrt{\frac{\gamma}{\pi t}}\, \mathrm{e}^{-\frac{\gamma(x-x_0)^2}{4t}} \ . \tag{62}$$

Problem 34. The initial temperature profile is given by the function $u(x) = u_0 e^{-(x/l_0)^2}$, $x \in (-\infty, \infty)$. Use the Green's function (62) to find $u(x,t)$.

Schrödinger equation

The Schrödinger equation ($\gamma = 2m/\hbar > 0$),

$$-i\gamma u_t = u_{xx} \ , \qquad\qquad x \in (-\infty, \infty) \tag{63}$$

is very close to (27), and the theory of its Green's function is quite similar to what has been done above. The result for G reads

$$G(x, x_0, t) \ = \ \frac{\mathrm{e}^{-i\pi/4}}{2}\sqrt{\frac{\gamma}{\pi t}}\, \mathrm{e}^{i\frac{\gamma(x-x_0)^2}{4t}} \ . \tag{64}$$

Problem 35. Derive Eq. (64). When finding the normalization constant, the following integral will be useful

$$\int_{-\infty}^{\infty} \mathrm{e}^{iy^2} dy = \sqrt{\pi}\, \mathrm{e}^{i\pi/4} \ . \tag{65}$$

Problem 36. The initial state of the one-dimensional quantum particle is given by the wavefunction $\psi(x) = Ae^{-(x/l_0)^2 + ikx}$, $x \in (-\infty, \infty)$, A is the normalization constant. Find $\psi(x,t)$ with the Green's function (64). With the solution found, determine the velocity of the packet and the evolution of the characteristic width of the packet. The following integral will be useful (a and b may be complex, provided either $\mathrm{Re}\, a > 0$, or $\mathrm{Re}\, a = \mathrm{Re}\, b = 0$).

$$\int_{-\infty}^{\infty} \mathrm{e}^{-ax^2+bx}\, dx = \sqrt{\frac{\pi}{a}}\, \mathrm{e}^{b^2/4a} . \tag{66}$$

This integral is an analytic function of a at $\mathrm{Re}\, a > 0$. Hence, the square root is *unambiguously* understood as $\sqrt{a} = \sqrt{|a|}\mathrm{e}^{i\varphi/2}$, where $a = |a|\, \mathrm{e}^{i\varphi}$, with $\varphi \in [-\pi/2, \pi/2]$.