Physics 605: Green Functions

Updated October 1, 2017

Suppose we want to solve the following equation in one dimension,

$$\left[\frac{\partial^2}{\partial x^2} - m^2\right]\phi(x) = f(x) \tag{1}$$

in the domain $0 \leq x < L$ and such that $\phi(0) = \phi(L) = 0$. Finally, assume $\langle f|g\rangle = \int_0^L dx\ f^*(x)g(x)$. For good measure, we will also assume that $f(x)$ belongs to the same Hilbert space – in other words, $f(0) = f(L) = 0$.

1 Defining the Green's function

We first seek to find the eigenfunctions of the operator, $\partial^2/\partial x^2 - m^2$, which is self-adjoint (proof not given) in our inner product. The eigenfunctions satisfy,

$$\left(\frac{\partial^2}{\partial x^2} - m^2\right)|\lambda\rangle = \lambda\,|\lambda\rangle\,. \tag{2}$$

The solutions of this equation are

$$|\lambda\rangle = A_\lambda \cos(\sqrt{\lambda + m^2}x) + B_\lambda \sin(\sqrt{\lambda + m^2}x), \tag{3}$$

where we note that λ can be negative and the square root can be imaginary. Finally, applying the boundary conditions yields $A_- = 0$ and $\lambda + m^2 = -\pi^2 n^2/L^2$. Thus, $\lambda = -(\pi^2 n^2/L^2 + m^2)$. Thus, we know that the functions

$$|n\rangle = \sqrt{\frac{2}{L}}\sin\left(\pi n x/L\right) \tag{4}$$

are the eigenfunctions of $\partial_x^2 - m^2$and the corresponding eigenvalues are $\lambda_n = -m^2 - (\pi n/L)^2$.

1.1 Eigenfunction expansion

Now we can solve Eq. (1) by expanding in eigenfunctions. In particular, we have

$$\phi(x) = \sum_{n=1}^{\infty} c_n\,|n\rangle\,. \tag{5}$$

Therefore,

$$c_n = \frac{\langle n|f\rangle}{-m^2 - (\pi n/L)^2} = \frac{1}{-m^2 - (\pi n/L)^2} \int_0^L dx \sqrt{\frac{2}{L}} \sin\left(\frac{\pi n x}{L}\right) f(x). \quad (6)$$

Putting this together, we find

$$|\phi\rangle = \sum_{n=1}^{\infty} |n\rangle \frac{\langle n|f\rangle}{\lambda_n}. \quad (7)$$

Let's rewrite this a bit:

$$\begin{aligned} |\phi\rangle &= \left[\sum_{n=1}^{\infty} \frac{|n\rangle \langle n|}{\lambda_n}\right] |f\rangle \\ &\equiv \mathcal{G}\,|f\rangle\,. \end{aligned} \quad (8)$$

The linear map $\mathcal{G}$ is called a **Green operator**. We can also express it as a function, a **Green's function** by

$$\begin{aligned} \phi(x) &= \int_0^L dx \sum_{n=1}^{\infty} \frac{-2}{L\,[m^2 + (\pi n/L)^2]} \sin\left(\frac{\pi n x}{L}\right) \sin\left(\frac{\pi n x''}{L}\right) f(x'') \\ &\equiv \int_0^L dx\; G(x, x'') f(x''). \end{aligned} \quad (9)$$

This gives us another way to find $G(x, x')$ – let $f(x'') = \delta(x'' - x')$. Then we find that

$$\phi(x) = G(x, x'). \quad (10)$$

In other words, the Green function satisfies this equation

$$\left[\partial_x^2 - m^2\right] G(x, x') = \delta(x - x'). \quad (11)$$

1.2 Direct computation

Now that we have Eq. (11), we can find a more direct solution for $G(x, x')$. In particular, integrate both sides of the equation in a region around x' to find

$$\int_{x'-\epsilon}^{x'+\epsilon} dx[\partial_x^2 - m^2]\phi = \partial_x \phi|_{x'-\epsilon}^{x'+\epsilon} - m^2 \mathcal{O}(\epsilon) = 1. \quad (12)$$

Taking $\epsilon \to 0$ concludes that $G(x, x')$ has a discontinuity in its first derivative precisely at x' and that

$$\lim_{\epsilon \to 0} \frac{\partial G}{\partial x}\bigg|_{x'-\epsilon}^{x'+\epsilon} = 1. \quad (13)$$

We can solve $G(x, x')$ in the region $0 \leq x < x'$ and $x' < x \leq L$ individually, then sew them together at x' according the Eq. (13).
Case $0 \leq x < x'$:

The general solutions are

$$G(x, x') = Ae^{mx} + Be^{-mx}. \tag{14}$$

Setting $G(x, x') = 0$ when $x = 0$ gives $G(x, x') = A_- \sinh(mx)$ for some constant A_-.

Case $x' < x \leq L$:

Setting $G(L, x') = 0$ we have $A = -Be^{-2mL}$. Therefore, $G(x, x') = A_+ e^{-mL} \sinh[m(L - x)]$. We can absorb the e^{-mL} into A_+ so that $G(x, x') = A_+ \sinh[m(L - x)]$.

Now we apply the boundary condition at $x = x'$. We also require that the function is continuous across x'. In other words,

$$\begin{aligned} -A_+ m \cosh[m(L - x')] - A_- m \cosh(mx') &= 1 \qquad (15) \\ A_+ \sinh[m(L - x')] - A_- \sinh[mx'] &= 0. \qquad (16) \end{aligned}$$

This gives us $A_+ = \sinh(mx')C$ and $A_- = \sinh[m(L - x')]C$ from the second equation. Consequently,

$$C = \frac{-m^{-1}}{\sinh(mx') \cosh[m(L - x')] + \cosh(mx') \sinh[m(L - x')]} = \frac{-m^{-1}}{\sinh(mL)}. \tag{17}$$

Therefore,

$$G(x, x') = -\frac{1}{m} \begin{cases} \frac{\sinh[m(L-x')] \sinh(mx)}{\sinh(mL)}, & x < x' \\ \frac{\sinh[m(L-x)] \sinh(mx')}{\sinh(mL)}, & x > x' \end{cases} \tag{18}$$

Thus, we now have two ways to write the same function! More to the point, this wacky expression is somehow equal to

$$G(x, x') = \sum_{n=1}^{\infty} \frac{2}{L\left[-m^2 - (\pi n/L)^2\right]} \sin\left(\frac{\pi n x}{L}\right) \sin\left(\frac{\pi n x'}{L}\right). \tag{19}$$

We also note here some notation, borrowed from Jackson. Let $x_< = \min(x, x')$ and $x_> = \max(x, x')$. Then we can write Eq. (18) into a single line as

$$G(x, x') = -\frac{1}{m} \frac{\sinh[m(L - x_>)] \sinh(mx_<)}{\sinh(mL)}. \tag{20}$$

This looks shorter but, to be clear, it is kind of a cheat. To use it, you have to decompress it back into something of the form of Eq. (18).

2 When is there a Green's function?

If we think about the Green's operator, $\mathcal{G}$, corresponding to a particular linear operator, $\mathcal{L}$, we see that

$$\mathcal{L}\mathcal{G} = 1, \tag{21}$$

or, in other words, the Green's operator is the formal inverse of the linear operator we are interested in. Since we know that

$$|\phi\rangle = \mathcal{G}\,|f\rangle \tag{22}$$

solves

$$\mathcal{L}\,|\phi\rangle = |f\rangle\,, \tag{23}$$

we can ask ourselves what must be true in order for a Green's function to exist.

First, the solution $|\phi\rangle$ must be uniquely defined. In finite-dimensional linear algebra, this would require ker $\mathcal{L}$, the set of vectors that $\mathcal{L}$ takes to 0, to be trivial. In this case, it means only the zero vector goes to zero. This is true so long as $\mathcal{L}$ has no zero eigenvalues. Note that if it did have zero eigenvalues, the expression defining $\mathcal{G}$,

$$\mathcal{G} = \sum_n \frac{|n\rangle\,\langle n|}{\lambda_n}$$

would not exist since λ_n would be zero for some n. Second, we require that if there is a state, $\langle w|$ such that $\langle w|\,\mathcal{L} = 0$, then $\langle w|f\rangle = 0$ as well. If $\mathcal{L}$ is self-adjoint, however, we see that

$$\langle w|\,\mathcal{L} = \langle w|\,\mathcal{L}^\dagger = (\mathcal{L}\,|w\rangle)^\dagger\,. \tag{24}$$

Thus, if $\mathcal{L}$ has no zero eigenvalues and is self-adjoint, there are no particular conditions that $|f\rangle$ would have to satisfy.

If both conditions are met, the operator $\mathcal{L}$ is invertible. An invertible operator also has another consequence: $\mathcal{L}\,|\phi\rangle = 0$ implies that $|\phi\rangle = 0$. This is exactly true for Laplace's equation.

3 Nontrivial boundaries

The Green's functions can also help us solve for functions with non-trivial boundary conditions. Consider a solution to

$$\left(\frac{\partial^2}{\partial x^2} - m^2\right)\phi(x) = f(x) \tag{25}$$

where $\phi(x)$ satisfies $\phi(0) = \phi_0$ and $\phi(L) = \phi_L$. Meanwhile, let $G(x, x')$ be the Green's function that vanishes at $x = 0$ and $x = L$. Compute

$$\int_0^L dx'\ G(x, x')\rho(x') = \int_0^L dx'\ G(x, x')\left(\frac{\partial^2}{\partial x'^2} - m^2\right)\phi(x'). \tag{26}$$

Integrating by parts twice gives

$$\begin{aligned}\int_0^L dx'\ G(x, x')\rho(x') &= G(x, x')\frac{\partial_x \phi(x')}{\partial x'}\bigg|_{x'=0}^{x'=L} - \frac{\partial G(x, x')}{\partial x'}\phi(x')\bigg|_{x'=0}^{x'=L} \\ &\quad + \int_0^L \delta(x - x')\phi(x'). \end{aligned} \tag{27}$$

The last term comes from the fact that $G(x, x')$ is a Green's function. Finally, we use the fact that $G(x, L) = G(x, 0) = 0$. This tells us

$$\phi(x) = \int_0^L dx'\ G(x, x')\rho(x') + \frac{\partial G(x, x')}{\partial x'}\phi(x')\bigg|_{x'=0}^{x'=L}. \tag{28}$$

The last term depends only on ϕ_0 and ϕ_L, the values of ϕ on the boundary. Hence, even when $\rho(x') = 0$ but the boundary conditions are not trivial, we see that we can use $G(x, x')$ and a proper Hilbert space to find the solution.

The generalization to Neumann boundary conditions, setting $\partial\phi/\partial x$ on the boundaries should be straightforward.

4 Poisson Equation and the Laplacian

4.1 Harmonic functions

A harmonic function is one that satisfies Laplace's equation. Harmonic functions have a number of interesting and important properties.

Theorem: If $\nabla^2\phi = 0$ and ϕ vanishes on the boundary of some domain, then $\phi = 0$.

To prove this, we first prove the **mean-value theorem** (this is slightly different than the mean-value theorem of regular calculus). That is,

$$\phi(\mathbf{r}) = \frac{1}{4\pi R^2} \int_{\partial R} dA' \phi(\mathbf{r} + \mathbf{r}'). \tag{29}$$

That is, the average of ϕ on a sphere of radius R around a point is equal to the value of ϕ on that point. To prove this lemma, we write

$$\int_{\mathcal{R}} d^3r \ \nabla^2 \phi = \int_{\partial \mathcal{R}} d\mathbf{A} \cdot \nabla \phi, \tag{30}$$

from the divergence theorem. We let $\mathcal{R}$ be the ball of radius R and $\partial\mathcal{R}$ its boundary (the sphere of radius R). Then

$$\begin{aligned} \int_{\mathcal{R}} d^3r \ \nabla^2 \phi &= \int_{\partial \mathcal{R}} dA \ \frac{\partial \phi}{\partial r} \\ &= \frac{\partial}{\partial r} \int_{\partial \mathcal{R}} dA \ \phi. \end{aligned} \tag{31}$$

Therefore, since the left hand side is zero since ϕ is harmonic

$$\int_{\partial \mathcal{R}} dA \ \phi(\mathbf{r})$$

is independent of the sphere's radius R. Now we compute what happens when we take the sphere's radius to zero. We find, then, that

$$\int_{\partial \mathcal{R}} \phi \to 4\pi R^2 \phi(\mathbf{r}), \tag{32}$$

where $\mathbf{r}$ is the center of the sphere. Therefore, we have the result of Eq. (29).

A consequence of the mean-value theorem is that harmonic functions take their maximum and minimum values on the boundary of their domain. This is called the **strong maximum** and **strong minimum** principle, respectively. If there was a maximum inside the domain, say at a point $\mathbf{r}_0$, we could surround it by a sphere of some finite radius. Then

$$\phi(\mathbf{r}_0) > \int_{\partial \mathcal{R}} dA \ \phi, \tag{33}$$

a clear violation of the mean-value theorem. Similarly, ϕ cannot have a minimum inside the domain.

Now we are in a position to prove our main theorem – when $\phi = 0$ on the boundary, the maximum and minimum values of ϕ must be 0. Hence, ϕ must be zero.

4.2 Poisson equation

The Poisson equation is

$$\nabla^2 \phi(\mathbf{r}) = 4\pi\rho(\mathbf{r}). \tag{34}$$

With appropriate boundary conditions, any solution of this equation can be written in terms of the solution to

$$\nabla^2 G(\mathbf{r}, \mathbf{r}') = 4\pi\delta^D(\mathbf{r} - \mathbf{r}'). \tag{35}$$

I put the 4π there for later convenience, and to match other textbooks.

In infinite space, with the boundary condition $\phi(\mathbf{r}) \to 0$ as $|\mathbf{r}| \to \infty$, the solution to this equation is

$$G(\mathbf{r}, \mathbf{r}') = \frac{1}{|\mathbf{r} - \mathbf{r}'|}. \tag{36}$$

This is the **Coulomb potential**. Then

$$\phi(\mathbf{r}) = \int d^D\mathbf{r}'\ G(\mathbf{r}, \mathbf{r}')\rho(\mathbf{r}') = \int d^D\mathbf{r}'\ \frac{\rho(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} \tag{37}$$

We can also divide space up into two regions, $|\mathbf{r}| < |\mathbf{r}'|$ and $|\mathbf{r}| > |\mathbf{r}'|$. In each of these regions, $\phi(\mathbf{r}) = 0$. Let's take each region in turn.

$|\mathbf{r}| < |\mathbf{r}'|$:

The solution of Laplace's equation can be written $\phi_<(\mathbf{r}) = \sum_{\ell=0}^{\infty} \sum_{m=-\infty}^{\infty} A_{\ell m} r^\ell Y_{lm}(\theta, \varphi)$. Consequently, we see that

$$\frac{1}{|\mathbf{r} - \mathbf{r}'|} = \sum_{\ell=0}^{\infty} \sum_{m=-\infty}^{\infty} A_{\ell m} r^\ell Y_{lm}(\theta, \varphi), \tag{38}$$

for some choice of $A_{\ell m}$.

$|\mathbf{r}| > |\mathbf{r}'|$:

The solution of Laplace's equation can be written $\phi_>(\mathbf{r}) = \sum_{\ell=0}^{\infty} \sum_{m=-\infty}^{\infty} B_{\ell m} r^{-\ell-1} Y_{lm}(\theta, \varphi)$. Consequently, we see that

$$\frac{1}{|\mathbf{r} - \mathbf{r}'|} = \sum_{\ell=0}^{\infty} \sum_{m=-\infty}^{\infty} B_{\ell m} r^{-\ell-1} Y_{lm}(\theta, \varphi), \tag{39}$$

for some choice of $B_{\ell m}$.

Precisely at $r = |\mathbf{r}'| \equiv r'$ we can set $\phi_< = \phi_>$. Therefore,

$$\sum_{\ell=0}^{\infty} \sum_{m=-\infty}^{\infty} \left[A_{\ell m}(r')^{\ell} - B_{\ell m}(r')^{-\ell-1}\right] Y_{\ell m}(\theta, \varphi) = 0. \tag{40}$$

The orthogonality of the $Y_{\ell m}$ tell us that $B_{\ell m} = A_{\ell m} r^{2\ell+1}$.

To see what the other boundary condition is for ϕ, we need to look more closely at the Dirac delta that appears. Let's rewrite $\delta^3(\mathbf{r})$ in spherical coordinates. We have

$$\delta^3(\mathbf{r} - \mathbf{r}') = \frac{1}{r^2 \sin\theta} \delta(r - r')\delta(\theta - \theta')\delta(\varphi - \varphi'). \tag{41}$$

It is easy to check that the integral of both sides always agree.

Let's integrate $\nabla^2 \phi = \delta^3(\mathbf{r})$ from $r' - \epsilon$ to $r' + \epsilon$. This gives

$$\left.\frac{\partial \phi}{\partial r}\right|_{r'-\epsilon}^{r'+\epsilon} = \frac{1}{r'^2 \sin\theta} \delta(\theta - \theta')\delta(\varphi - \varphi'). \tag{42}$$

Therefore, the derivative of ϕ has a discontinuity at a single point (θ', φ') on the sphere. We then obtain

$$\begin{aligned} \frac{1}{(r')^2} \frac{\delta(\theta - \theta')\delta(\varphi - \varphi')}{\sin\theta} &= \sum_{\ell=0}^{\infty} \sum_{m=-\infty}^{\infty} \left[A_{\ell m} \ell (r')^{\ell-1} + B_{\ell m}(\ell+1)(r')^{-\ell-2}\right] Y_{\ell m}(\theta, \varphi) \\ \to \frac{\delta(\theta - \theta')\delta(\varphi - \varphi')}{\sin\theta} &= \sum_{\ell=0}^{\infty} \sum_{m=-\infty}^{\infty} A_{\ell m}(2\ell+1)(r')^{\ell+1} Y_{\ell m}(\theta, \varphi). \end{aligned} \tag{43}$$

We can finish off the calculation using the completeness relation for the $Y_{\ell m}$. In particular, we have that

$$\sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} Y_{\ell m}(\theta, \varphi) Y^*_{\ell m}(\theta', \varphi') \frac{2\ell+1}{4\pi} = \frac{\delta(\theta - \theta')\delta(\varphi - \varphi')}{\sin\theta}. \tag{44}$$

Setting this equation equal to our expansion in terms of $A_{\ell m}$ and matching term by term gives $A_{\ell m} = \frac{(r')^{-\ell-1}}{4\pi} Y^*_{\ell m}(\theta', \varphi')$. This gives, finally,

$$\phi = \sum_{\ell=0}^{\infty} \sum_{m=-\infty}^{\infty} Y_{\ell m}(\theta, \phi) Y^*_{\ell m}(\theta', \varphi') \begin{cases} \frac{1}{4\pi} \frac{r^{\ell}}{(r')^{\ell+1}} & r < r' \\ \frac{1}{4\pi} \frac{(r')^{\ell}}{r^{\ell+1}} & r > r' \end{cases} \tag{45}$$

This gives the expression for the Green's function as an expansion in spherical harmonics. The expansion for $r > r'$ is called the multipole expansion.

4.3 Multipole Expansion

Another way to perform the expansion is to assume that $r' \ll r$ and expand the Coulomb potential directly. In other words,

$$\begin{aligned} \frac{1}{|\mathbf{r}-\mathbf{r}'|} &= \frac{1}{\sqrt{r^2+r'^2-2rr'\cos(\theta-\theta')}} = \frac{1}{r}\frac{1}{\sqrt{1-2(r'/r)\cos(\theta-\theta')+(r'/r)^2}} \\ &= \frac{1}{r}+\frac{r'\cos(\theta-\theta')}{r^2}+\cdots . \end{aligned} \tag{46}$$

The first term is the monopole term, the second is called the dipole term, the third the quadrupole term, and so on.

For arbitrary charge distributions, we find out that

$$\phi(\mathbf{r}) = \sum_{\ell=0}^{\infty}\sum_{m=-\ell}^{\ell}\frac{1}{r^{\ell+1}}Y_{\ell m}(\theta,\varphi)\int d\Omega'\ \frac{1}{4\pi}Y^*_{\ell m}(\theta',\varphi')(r')^{\ell}\rho(r',\theta',\varphi'), \tag{47}$$

where $d\Omega' = dr'd\theta'd\varphi'\ (r')^2\sin(\theta')$.

Yet another alternative method of deriving the multipole expansion would be to directly expand $1/|\mathbf{r}-\mathbf{r}'|$ in powers of $\mathbf{r}$. We can do this explicitly by

$$\begin{aligned} \frac{1}{|\mathbf{r}-\mathbf{r}'|} &= \frac{1}{|\mathbf{r}|}\frac{1}{\sqrt{1+(\mathbf{r}')^2/\mathbf{r}^2-2\mathbf{r}'\cdot\mathbf{r}/(\mathbf{r})^2}} \\ &= \frac{1}{|\mathbf{r}|}+\frac{\mathbf{r}'\cdot\mathbf{r}}{|\mathbf{r}|^3}+\frac{3(\mathbf{r}'\cdot\mathbf{r})^2-(\mathbf{r})^2(\mathbf{r}')^2}{2|\mathbf{r}|^5}+\cdots \end{aligned} \tag{48}$$

Putting this together, we obtain

$$\begin{aligned} \phi(\mathbf{r}) &= \frac{1}{|\mathbf{r}|}\int_V d^3r'\ \rho(\mathbf{r}')+\frac{\mathbf{r}}{|\mathbf{r}|^3}\cdot\int_V d^3r'\ \mathbf{r}'\rho(\mathbf{r}') \\ &\quad +\frac{\mathbf{r}_i\mathbf{r}_j}{|\mathbf{r}|^5}\int_V d^3r\ \frac{3\mathbf{r}_i'\mathbf{r}_j'-\delta_{ij}(\mathbf{r}')^2}{2}\rho(\mathbf{r}')+\cdots . \end{aligned} \tag{49}$$

Let's give these coefficients names so we can study them further. We'll write

$$\begin{aligned} q &= \int_V d^3r'\ \rho(\mathbf{r}') \\ \mathbf{p} &= \int_V d^3r'\ \mathbf{r}'\rho(\mathbf{r}') \\ Q_{ij} &= \int_V d^3r'\ \frac{3r_i'r_j'-\delta_{ij}(\mathbf{r}')^2}{2}\rho(\mathbf{r}'). \end{aligned} \tag{50}$$

Therefore,

$$\phi(\mathbf{r}) = \frac{q}{|\mathbf{r}|}+\frac{1}{|\mathbf{r}|^2}\hat{\mathbf{r}}\cdot\mathbf{p}+\cdots . \tag{51}$$

Now let's write these using spherical harmonics to finally complete the multipole expansion circle. Since $Y_{00} = 1/\sqrt{4\pi}$, $q = \sqrt{4\pi} q Y_{00}(\theta, \varphi)$. For the dipole term, we know that $\hat{\mathbf{r}} = \sin\theta\cos\varphi\hat{\mathbf{x}} + \sin\theta\sin\varphi\hat{\mathbf{y}} + \cos\theta\hat{\mathbf{z}}$ so that

$$\begin{aligned}\hat{\mathbf{r}} \cdot \mathbf{p} &= \sin\theta\cos\varphi p_x + \sin\theta\sin\varphi p_y + \cos\theta p_z \\ &= \sqrt{\frac{2\pi}{3}}\left[Y_{1,-1}(\theta,\varphi)(p_x - ip_y) + Y_{1,1}(\theta,\varphi)(p_x + ip_y) + \sqrt{2}Y_{1,0}(\theta,\varphi)p_z\right].\end{aligned}$$

Notice that there are 3 Y_{1m} and 3 components of $\mathbf{p}$. If we look at the quadrupole term, we see that Q_{ij} is a symmetric, traceless tensor, which has 5 independent components. There are also 5 Y_{2m} so we see that there are precisely enough Y_{2m} to expand $Q_{ij}\hat{\mathbf{r}}^i\hat{\mathbf{r}}^j$ into spherical harmonics. Since Q_{ij} is symmetric and traceless, it can be diagonalized. It's eigenvalues are, therefore, q_1, q_2 and $-q_1 - q_2$.

If $q_1 \neq q_2$ then the three eigenvectors are orthogonal and Q_{ij} selects a frame of axes in space. This is called **biaxial** symmetry. If $q_1 = q_2$ then Q_{ij} favors the third eigenvector, which is perpendicular to the other two. This is called **uniaxial** symmetry, since it selects a single axis. Note that, since eigenvectors are only unique up to magnitude, a uniaxial Q_{ij} selects an axis in space but not a direction!

4.4 Method of images

Let's consider the problem of solving

$$\nabla^2 G(\mathbf{r}, \mathbf{r}') = 4\pi\delta^3(\mathbf{r} - \mathbf{r}') \tag{52}$$

in the positive half space $z > 0$ with the boundary condition that $G = 0$ when $z = 0$. We also assume that $\phi(\mathbf{r}) \to 0$ as $|\mathbf{r}| \to \infty$.

We're going to derive a solution to this problem by taking advantage of the one we already have. In order to make our solution work, however, we need to prove something about the Laplacian that hasn't quite come up before.

Theorem: A solution to Laplace's equation in a domain $\mathcal{D}$ for which $\phi(\mathbf{r})$ is specified on the boundary $\partial\mathcal{D}$ is unique.

> Suppose there were two solutions, ϕ_1 and ϕ_2, sharing the same boundary condition on $\partial\mathcal{D}$. Then $\phi = \phi_1 - \phi_2$ would also be a solution with $\phi = 0$ on $\partial\mathcal{D}$. What we really want to prove, then,

is that $\phi = 0$ on $\partial\mathcal{D}$ implies it is zero throughout $\mathcal{D}$. If so, then $\phi_1 = \phi_2$ and we would have uniqueness.

To prove this last part, consider $\nabla(\phi\nabla\phi) = (\nabla\phi)^2 + \phi\nabla^2\phi$. Since $\nabla^2\phi = 0$ by construction, we have $\nabla(\phi\nabla\phi) = (\nabla\phi)^2$. Integrating both sides over volume and using the divergence theorem on the left side, we obtain

$$\oint_{\partial\mathcal{D}} d\mathbf{a}\cdot\nabla\phi\ \phi = \int_{\mathcal{D}} dV\ (\nabla\phi)^2. \tag{53}$$

The boundary condition we derived for ϕ implies that the left hand side is zero. Therefore, the right hand side must be as well. Since the integrand is always positive or zero, it must be zero. Therefore, we obtain the result that ϕ must be constant and, since it is zero on the boundary, it must be zero everywhere.

Uniqueness helps us because of the following fact:

$$\phi = \frac{1}{|\mathbf{r} - x'\hat{\mathbf{x}} + y'\hat{\mathbf{y}} + z'\hat{\mathbf{z}}|} - \frac{1}{|\mathbf{r} - x'\hat{\mathbf{x}} + y'\hat{\mathbf{y}} - z'\hat{\mathbf{z}}|} \tag{54}$$

vanishes on the $z = 0$ plane. Consequently, when $z > 0$, it solves the Poisson equation with precisely the boundary condition we want. Since the solution is unique, we can stop looking for solutions.

Indeed, if $G(x - x', y - y', z - z')$ is a Green function whose arguments are even, then $G(x - x', y - y', z - z') - G(x - x', y - y', z + z')$ always vanishes on the $z = 0$ plane. The method of images turns out to be useful in many different linear equations!

4.5 Laplacian in 2D

It is interesting to compute the Green function in 2D for the Poisson equation. In that case, we have

$$\nabla^2 G(\mathbf{r}, \mathbf{r}') = 4\pi\delta^2(\mathbf{r} - \mathbf{r}'). \tag{55}$$

When $\mathbf{r}' = 0$, the solution is rotationally symmetric outside of the origin. It suffices to solve $\nabla^2\phi = 0$ for $|\mathbf{r}| > 0$. The only axisymmetric solutions are $\phi = A\ln(|\mathbf{r}|/R)$, where R is some constant. Notice that $\phi = -\ln R + A\ln r =$ constant $+ A\ln r$ which are just the two linearly independent axisymmetric solutions we already know and "love."

To set A, we note that $\oint ds\, \hat{\mathbf{r}} \cdot \nabla\phi = 4\pi$ which tells us that $A = 4\pi$. Finally, we take advantage of the fact that, if $\phi(\mathbf{r})$ solves Laplace's equation then $\phi(\mathbf{r}+\mathbf{v})$ also does for constant vector $\mathbf{v}$. This tells us, finally, that

$$G(\mathbf{r}, \mathbf{r}') = 4\pi \ln(|\mathbf{r} - \mathbf{r}'|/R). \tag{56}$$

5 Time-dependent Green functions

5.1 The diffusion equation

Consider the diffusion equation,

$$\frac{\partial n}{\partial t} = D\frac{\partial^2 n}{\partial x^2}. \tag{57}$$

We wish to obtain the solution subject to the *initial* condition $n(x, 0) = \delta(x-x')$. Why? Let $G(x, x'; t)$ solve the diffusion equation with $G(x, x'; 0) = \delta(x - x')$. Then

$$n(x,t) = \int_0^L dx'\; f(x')G(x, x'; t) \tag{58}$$

solves the diffusion equation with $n(x, 0) = f(x)$. To see this, let's just apply the diffusion equation to the expression in Eq. (58). Therefore,

$$\left[\frac{\partial}{\partial t} - D\frac{\partial^2}{\partial x^2}\right] n(x,t) = \int_0^L dx' f(x') \left[\frac{\partial}{\partial t} - D\frac{\partial^2}{\partial x^2}\right] G(x, x', t) = 0. \tag{59}$$

In addition, $n(x, 0) = \int_0^L dx'\; f(x')\delta(x - x') = f(x)$.

In fact, this is a Green function exactly as we have already discussed them. Consider the equation

$$\left[\frac{\partial}{\partial t} - D\frac{\partial^2}{\partial x^2}\right] n(x,t) = f(x)\delta(t) \tag{60}$$

with $n(x, t) = 0$ for $t < 0$. Then integrating with respect to t from $-\epsilon$ to ϵ ($\epsilon > 0$) gives

$$n(x, \epsilon) - n(x, -\epsilon) = n(x, \epsilon) = f(x). \tag{61}$$

Taking $\epsilon \to 0$ gives us the result we want. Now all that remains is to solve the equation.

This is a good opportunity for us to use Laplace or Fourier transforms. But as we haven't talked about those yet, we'll look for another method of solution. Instead, let us first notice that we can translate solutions to obtain new solutions so that it is sufficient to consider the case that $x' = 0$. Secondly, notice that if I have a solution to the diffusion equation, $n(x,t)$, then $s^{-1}n(sx, s^2t)$ is also a solution. To prove this, just invent new variables, $\tilde{x} = sx$ and $\tilde{t} = s^2 t$. This tells us that

$$s^2 \left[\frac{\partial}{\partial \tilde{t}} - D \frac{\partial^2}{\partial \tilde{x}^2} \right] n(\tilde{x}, \tilde{t}) = \delta(x)\delta(t). \tag{62}$$

On the right hand side, we have $\delta(x)\delta(t) = s^3 \delta(sx)\delta(s^2 t)$. Therefore, the left and right hand sides are equal when $n \to n/s^{-1}$ as well.

There is one conclusion from this:

$$n(x,t) = \frac{1}{\sqrt{t}} f\left(D^{-1/2} \frac{x}{\sqrt{t}} \right). \tag{63}$$

Now that we know this, we can put our ansatz back into the equation. Therefore,

$$\begin{aligned} \frac{\partial n}{\partial t} &= -\frac{1}{2t^{3/2}} f(D^{-1/2}x/\sqrt{t}) - D^{-1/2}\frac{x}{2t^2} f'(D^{-1/2}x/\sqrt{t}) & (64) \\ \frac{\partial^2 n}{\partial x^2} &= \frac{1}{t^{3/2}D} f''(D^{-1/2}x/\sqrt{t}). & (65) \end{aligned}$$

Therefore,

$$\left[\frac{\partial}{\partial t} - D \frac{\partial^2}{\partial x^2} \right] n(x,t) = -t^{-3/2} \left[f''(D^{-1/2}x/\sqrt{t}) + \frac{x}{\sqrt{t}} f'(D^{-1/2}x/\sqrt{t}) + f(D^{-1/2}x/\sqrt{t}) \right]. \tag{66}$$

For any finite $t > 0$, the result in brackets must also be zero. Let's call $\xi = D^{-1/2}x/\sqrt{t}$. Then the equation we really want to solve is a one-dimensional ODE,

$$f''(\xi) + \xi f'(\xi) + f(\xi) = 0. \tag{67}$$

As it happens, this equation can be re-arranged further and solved. Notice that

$$W^{-1}(\xi) \left[W(\xi) f'(\xi) \right]' = \frac{W'(\xi)}{W(\xi)} f'(\xi) + f''(\xi). \tag{68}$$

Let $W'(\xi)/W(\xi) = \xi$ so that $W(\xi) = e^{\xi^2/2}$. Therefore, our equation can be rewritten as

$$\left[e^{\xi^2/2} f'(\xi) \right]' + f(\xi) e^{\xi^2/2} = 0. \tag{69}$$

Let $g(\xi) = f(\xi)e^{\xi^2/2}$. Then $g'(\xi) = f'(\xi)e^{\xi^2/2} + \xi g(\xi)$. Rewriting our equation in terms of $g(\xi)$ then gives

$$\left[g'(\xi) - \xi g(\xi) \right]' + g(\xi) = g'' - \xi g'(\xi) = 0. \tag{70}$$

Finally, we have an equation we can solve. Notice that it can be rearranged to

$$\frac{g''}{g'} = \xi \to (\ln g')' = \xi \to g' = e^{\xi^2/2} \to g(\xi) = C + \int_0^\xi d\eta e^{\eta^2/2}. \tag{71}$$

Incidentally, the function $\int_0^\xi d\eta e^{\eta^2} = \sqrt{\pi/4}\mathrm{erfi}(\xi)$.

Putting everything back together, we conclude that

$$f(\xi) = e^{-\xi^2/2}\left[C + \frac{2}{\sqrt{\pi}}\mathrm{erfi}(\xi/\sqrt{2})\right] \tag{72}$$

and

$$n(x,t) = \frac{C_1}{t^{1/2}}e^{-x^2/(2Dt)} + \frac{C_2}{t^{1/2}}e^{-x^2/(2Dt)}\mathrm{erfi}\left(\frac{x}{\sqrt{2Dt}}\right). \tag{73}$$

Though this is the most general solution, it does not necessarily satisfy our initial conditions. Indeed, notice that $\mathrm{erfi}(-\eta) = -\mathrm{erfi}(\eta)$. Since our initial data is symmetric, we conclude that $C_2 = 0$. Moreover, we can consider the integral of $n(x,0)$ with respect to x. This gives

$$\int_\infty^\infty dx\ n(x,0) = 1 = \frac{C_1}{\sqrt{t}}\int_{-\infty}^\infty dx\ e^{-x^2/(2Dt)} = C_1\sqrt{2\pi D}. \tag{74}$$

Therefore, we must have

$$n(x,t) = \frac{1}{\sqrt{2\pi Dt}}\exp\left[-\frac{x^2}{2Dt}\right]. \tag{75}$$

Therefore, the Green function is

$$G(x-x';t) = \frac{1}{\sqrt{2\pi Dt}}\exp\left[-\frac{(x-x')^2}{2Dt}\right]. \tag{76}$$

5.2 Intermediate-time asymptotics

The general solution of the diffusion equation for any initial condition is

$$n(x,t) = \frac{1}{\sqrt{2\pi Dt}}\int_{-\infty}^\infty dx' \exp\left[-\frac{(x-x')^2}{2Dt}\right]n(x',0). \tag{77}$$

Suppose $n(x,0)$ is localized to a finite region between $-W \le x \le W$.

In the limit that $t \to \infty$, clearly $n(x,t) \to 0$. But what about for finite times that are still very long? Consider the case that $\sqrt{2Dt} \gg 2W$. Then the Green function varies more slowly than the function $n(x',0)$. In that case, we an expand the Green function in powers of x' – essentially a multipole expansion for the diffusion equation. We find

$$n(x,t) = G(x,0;t)\int_{-\infty}^{\infty} dx' n(x',0) + \partial_{x'} G(x,x';t)|_{x'=0}\int_{-\infty}^{\infty} dx'\ x' n(x',0) + \cdots . \tag{78}$$

The first term is the dominant term and implies

$$n(x,t) \approx \frac{1}{\sqrt{2\pi D t}} e^{-x^2/(2Dt)} N, \tag{79}$$

where $N = \int_{-\infty}^{\infty} dx' n(x',0)$. (Check that the next term is actually smaller than the first when $2Dt \gg 2W$).

Thus, the time evolution of any localized distribution of particles eventually approximates the Green function.

6 Wave equation

Another computation of interest is the Green function for the wave equation. Because we can specify the initial value and initial time derivative of any solution, there is some issue about what equation the Green function should really satisfy. If the Green function satisfies

$$\left[\frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \frac{\partial^2}{\partial x^2}\right] G(x,t;x',t') = \delta(x-x')\delta(t-t') \tag{80}$$

then we can obtain the relevant initial condition by integrating with respect to t from $t'-\epsilon$ to $t'+\epsilon$. This gives

$$\left.\frac{\partial G(x,t;x',t')}{\partial t}\right|_{t'-\epsilon}^{t'+\epsilon} = \delta(x-x'). \tag{81}$$

We also insist that $G(x,t;x',t')$ is continuous across t'.

6.1 Expansion in orthogonal functions

Suppose that we have boundary conditions $G(0,t;x',t') = G(L,t;x',t') = 0$. The Hilbert space is spanned by the orthonormal basis $|n\rangle = \sqrt{2/L}\sin(\pi n x/L)$.

Using $\sum_{n=1}^{\infty} |n\rangle\langle n| = \delta(x-x')$, we have the completeness relation

$$\sum_{n=1}^{\infty} \frac{2}{L}\sin\left(\frac{\pi n x}{L}\right)\sin\left(\frac{\pi n x'}{L}\right) = \delta(x-x'). \tag{82}$$

This allows us to expand $G(x, t; x', t') = \sum_n G_n(t; x', t') \, |n\rangle$ to obtain

$$\frac{1}{c^2} \frac{\partial^2 G_n}{\partial t^2} + \left(\frac{\pi n}{L}\right)^2 G_n = \sqrt{\frac{2}{L}} \sin\left(\frac{\pi n x'}{L}\right) \delta(t - t'). \tag{83}$$

Integrating both sides with respect to t tells us that

$$\frac{1}{c^2} \frac{\partial G_n}{\partial t}\bigg|_{t'-\epsilon}^{t'+\epsilon} = \sqrt{\frac{2}{L}} \sin\left(\frac{\pi n x'}{L}\right). \tag{84}$$

We also assume that G_n is continuous across t'.

The Green function is then

$$G_n = \begin{cases} A_- \sin\left(\frac{c\pi n t}{L} + \phi_-\right), & t < t' \\ A_+ \sin\left(\frac{c\pi n x}{L} + \phi_-\right), & t > t' \end{cases} \tag{85}$$

The continuity of G_n requires $A_- \sin(c\pi n t'/L + \phi_-) = A_+ \sin(c\pi n t'/L + \phi_+)$. Therefore,

$$\begin{aligned} A_+ \sin(c\pi n t'/L + \phi_+) - A_- \cos(c\pi n t'/L + \phi_-) &= 0 \\ A_+ \cos(c\pi n t'/L + \phi_+) - A_- \cos(c\pi n t'/L + \phi_-) &= \frac{2}{c\pi n} \sin(\pi n x'/L). \end{aligned}$$

Something seems off here, though. There are four unknowns and only two equations. To fix this, we assume that $G_n = 0$ when $t < t'$ – that a disturbance at time $t > t'$ cannot affect the shape of G at earlier times. Then the equations become

$$\begin{aligned} A_+ \sin(c\pi n t'/L + \phi_+) &= 0 \\ A_+ \cos(c\pi n t'/L + \phi_+) &= \frac{\sqrt{L/2}}{c\pi n} \sin(\pi n x'/L). \end{aligned}$$

These, now, have a unique solution. To solve the first equation, we let $\phi_+ = -c\pi n t'/L$, which implies

$$A_+ = \frac{\sqrt{2/L} \sin(\pi n x'/L)}{c\pi n}. \tag{86}$$

Finally,

$$G(x, t; x', t') = \sum_{n=1}^{\infty} \frac{2 \sin(\pi n x'/L) \sin(\pi n x/L)}{c\pi n L} \sin[c\pi n(t - t')/L]. \tag{87}$$

6.2 Using Characteristics

In an infinite domain, our current methods do not quite work (we'll fix this later in the class). However, we also know that the general solution to the wave equation is $G(x,t;x',t') = f(x-ct;x',t') + g(x+ct;x',t')$. The initial conditions give us

$$\begin{aligned} G(x,0;x',t') &= f(x;x',t') + g(x;x',t') \\ \partial_t G(x,t;x',t')|_{t=0} &= cg'(x;x',t') - cf'(x;x',t'). \end{aligned} \tag{88}$$

The initial conditions of the wave equation for the Green function tells us that

$$\begin{aligned} g(x;x',t') + f(x;x',t') &= 0 \\ g'(x;x',t') - f'(x;x',t') &= \frac{1}{c}\delta(x-x') \\ &\rightarrow \; g'(x;x',t') = \frac{1}{2c}\delta(x-x'). \end{aligned}$$

To finish, we need the indefinite integral of a Dirac delta. This is

$$\int_0^x dz\delta(z-x') = \Theta(x-x'), \tag{89}$$

where Θ is the Heaviside step function which equals 1 when its argument is positive and zero otherwise.

Therefore, we can write the Green function as

$$G(x,t;x',t') = \frac{1}{2c}\Theta[x-x'+c(t-t')] - \frac{1}{2c}\Theta[x-x'-c(t-t')]. \tag{90}$$

When we have some more mathematics under our belt, we will work out the Green function for the wave equation in 3D. For now, consider the case that $x' = 0$ and $t' = 0$. Then we see that $G = 1/(2c)$ when $x + ct > 0$ but $x - ct < 0$, and is zero otherwise. Graphically, this implies that the Green function is only nonzero in the shaded region of Fig. 1.

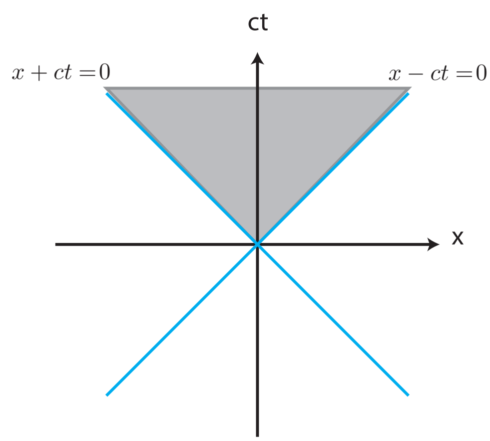

Figure 1: Space-time diagram for the one-dimensional wave equation.