

Unit 2-1-S: Supplementary Material - Green's Identities, Uniqueness, Dirichlet and Neumann Green's Function

Green's Identities

We want to show that the boundary value problem we have been discussing is well posed – that there is a unique solution. We start by deriving some results of vector calculus known as Green's Identities.

Consider

$$\int_V d^3r \nabla \cdot \mathbf{A} = \oint_S da \hat{\mathbf{n}} \cdot \mathbf{A} \quad \text{Gauss' Theorem} \quad (2.1.S.1)$$

Apply this to $\mathbf{A} = \phi \nabla \psi$ where ϕ and ψ are any two scalar functions. We get

$$\nabla \cdot \mathbf{A} = \phi \nabla^2 \psi + \nabla \phi \cdot \nabla \psi \quad \text{and also} \quad \hat{\mathbf{n}} \cdot \mathbf{A} = \phi \hat{\mathbf{n}} \cdot \nabla \psi = \phi \frac{\partial \psi}{\partial n} \quad (2.1.S.2)$$

Insert into Gauss' Theorem to get

$$\boxed{\int_V d^3r (\phi \nabla^2 \psi + \nabla \phi \cdot \nabla \psi) = \oint_S da \phi \frac{\partial \psi}{\partial n} \quad - \text{this is known as Green's 1st identity}} \quad (2.1.S.3)$$

Now let $\phi \leftrightarrow \psi$ in the above to get

$$\int_V d^3r (\psi \nabla^2 \phi + \nabla \psi \cdot \nabla \phi) = \oint_S da \psi \frac{\partial \phi}{\partial n} \quad (2.1.S.4)$$

Subtract the above two equations to get

$$\boxed{\int_V d^3r (\phi \nabla^2 \psi - \psi \nabla^2 \phi) = \oint_S da \left(\phi \frac{\partial \psi}{\partial n} - \psi \frac{\partial \phi}{\partial n} \right) \quad - \text{this is known as Green's 2nd identity}} \quad (2.1.S.5)$$

Now take $\psi(\mathbf{r}') = \frac{1}{|\mathbf{r} - \mathbf{r}'|}$, and $\phi(\mathbf{r}')$ to be the scalar potential so that $\nabla'^2 \phi(\mathbf{r}') = -4\pi\rho(\mathbf{r}')$, and lastly we will use that $\nabla^2 \psi = \nabla'^2 \psi = -4\pi\delta(\mathbf{r} - \mathbf{r}')$. Substitute these into Green's 2nd identity with \mathbf{r}' as the integration variable,

$$\int_V d^3r' \left[\phi(\mathbf{r}') [-4\pi\delta(\mathbf{r} - \mathbf{r}')] - \frac{1}{|\mathbf{r} - \mathbf{r}'|} [-4\pi\rho(\mathbf{r}')] \right] = \oint_S da' \left[\phi(\mathbf{r}') \frac{\partial}{\partial n'} \left(\frac{1}{|\mathbf{r} - \mathbf{r}'|} \right) - \frac{1}{|\mathbf{r} - \mathbf{r}'|} \frac{\partial \phi(\mathbf{r}')}{\partial n'} \right] \quad (2.1.S.6)$$

If \mathbf{r} lies within the volume V , then doing the integration over the delta function gives,

$$\phi(\mathbf{r}) = \int_V d^3r' \frac{\rho(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} + \oint_S \frac{da'}{4\pi} \left[\frac{1}{|\mathbf{r} - \mathbf{r}'|} \frac{\partial \phi(\mathbf{r}')}{\partial n'} - \phi(\mathbf{r}') \frac{\partial}{\partial n'} \left(\frac{1}{|\mathbf{r} - \mathbf{r}'|} \right) \right] \quad \mathbf{r} \text{ inside } V \quad (2.1.S.7)$$

But if \mathbf{r} lies outside the volume V , then one gets,

$$0 = \int_V d^3r' \frac{\rho(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} + \oint_S \frac{da'}{4\pi} \left[\frac{1}{|\mathbf{r} - \mathbf{r}'|} \frac{\partial \phi(\mathbf{r}')}{\partial n'} - \phi(\mathbf{r}') \frac{\partial}{\partial n'} \left(\frac{1}{|\mathbf{r} - \mathbf{r}'|} \right) \right] \quad \mathbf{r} \text{ outside } V \quad (2.1.S.8)$$

In the above expressions, the volume integral looks just like the usual Coulomb integral that gives the potential in terms of the charge density ρ . The first term in the surface integral looks like a similar Coulomb integral, but for a surface charge density $\sigma = (1/4\pi)(\partial\phi/\partial n)$. The second term in the surface integral gives the potential from a surface dipole layer of dipole strength $\phi/4\pi$. One can think of a surface dipole layer as follows: two infinitesimally thin locally parallel surfaces, separated by a distance d , one with surface charge density $+\sigma$ and the other with surface charge density $-\sigma$. Then take $d \rightarrow 0$ keeping $d\sigma$ finite.

Consider now Eq. (2.1.S.7). If we take the surface S off to infinity, so the V is the entire universe, and $E \sim \partial\phi/\partial n \rightarrow 0$ faster than $1/r$, then the surface integral will vanish and we recover the familiar Coulomb's Law,

$$\phi(\mathbf{r}) = \int_V d^3r' \frac{\rho(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} \quad \text{when } S \rightarrow \infty \quad (2.1.S.9)$$

So Eq. (2.1.S.7) therefore gives the generalization of Coulomb's Law when one is dealing with a system contained within a finite boundary.

For a *charge free* volume with $\rho(\mathbf{r}) = 0$ in V , the potential everywhere is determined by the potential and its normal derivative on the surface. But note, one cannot in general freely specify *both* ϕ and $\partial\phi/\partial n$ on the boundary surface, since the resulting ϕ computed by Eq. (2.1.S.7) for \mathbf{r} in V would not in general obey Laplace's equation $\nabla^2\phi(\mathbf{r}) = 0$ in V , nor would the right hand side of Eq. (2.1.S.8) in general vanish for \mathbf{r} outside V . The condition that ϕ must be a harmonic function in V , with $\nabla^2\phi = 0$, thus implies there must be some relation between ϕ and $\partial\phi/\partial n$ on the bounding surface.

Specifying ϕ on the surface is known as the Dirichlet boundary condition. Specifying $\partial\phi/\partial n$ on the surface is known as the Neumann boundary condition. Specifying both ϕ and $\partial\phi/\partial n$ on the surface is known as the Cauchy boundary condition. For Laplace's equation, the Cauchy boundary condition overspecifies the problem and a solution cannot in general be found.

Uniqueness of Solution to Poisson's Equation

If we have a system of charges of charges in a volume V bounded by a surface S , and we know *either* the potential ϕ or its normal derivative $\partial\phi/\partial n$ on the surface S , then there is a unique solution to Poisson's equation in the volume V .

proof:

Suppose we had two solutions ϕ_1 and ϕ_2 , both satisfying $\nabla^2\phi = -4\pi\rho$ inside V , and obeying the same boundary condition on S . Then define

$$U = \phi_2 - \phi_1 \quad \Rightarrow \quad \nabla^2 U = 0 \quad \text{inside } V \quad (2.1.S.10)$$

and

$$U = 0 \quad \text{on } S \quad \text{if one has Dirichlet boundary conditions, or} \\ \frac{\partial U}{\partial n} = 0 \quad \text{on } S \quad \text{if one has Neumann boundary conditions} \quad (2.1.S.11)$$

Use Green's 1st identity with $\phi = \psi = U$ to get

$$\int_V d^3r (U\nabla^2 U + \nabla U \cdot \nabla U) = \oint_S da U \frac{\partial U}{\partial n} \quad (2.1.S.12)$$

But $\nabla^2 U = 0$ by Eq. (2.1.S.10), and the surface integral also vanishes since either $U = 0$ or $\partial U/\partial n = 0$ on S . We are then left with,

$$\int_V d^3r |\nabla U|^2 = 0 \quad \Rightarrow \quad \nabla U = 0 \quad \Rightarrow \quad U = \text{constant} \quad (2.1.S.13)$$

For Dirichlet boundary conditions, since $U = 0$ on S , then the above constant must vanish and $U = 0$ everywhere in V . Thus $\phi_1 = \phi_2$ and the solution is unique.

For Neumann boundary conditions, ϕ_1 and ϕ_2 can only differ by only an arbitrary constant. Since $\mathbf{E} = -\nabla\phi$, the electric fields $\mathbf{E}_1 = -\nabla\phi_1$ and $\mathbf{E}_2 = -\nabla\phi_2$ will be equal. Hence the solution for ϕ is unique within an overall additive constant.

If the boundary S consists of several disjoint pieces, then the solutions is unique if one specifies ϕ on some pieces of S and $\partial\phi/\partial n$ on the other pieces.

A solution of Poisson's equation with *both* ϕ and $\partial\phi/\partial n$ specified on the same surface S (i.e. the Cauchy boundary condition) does not in general exist because we have just shown that specifying *either* ϕ or $\partial\phi/\partial n$ alone is sufficient to give a unique solution.

Green's Function for the Dirichlet Boundary Condition

We have previously discussed the idea of the Green's function. For the Coulomb problem, the Green's function $G(\mathbf{r}, \mathbf{r}')$ is the potential at position \mathbf{r} due to a point charge of unit magnitude at position \mathbf{r}' , so $\nabla^2 G(\mathbf{r}, \mathbf{r}') = -4\pi\delta(\mathbf{r} - \mathbf{r}')$. If we know $G(\mathbf{r}, \mathbf{r}')$ then we can find the potential $\phi(\mathbf{r})$ for any distribution of charges $\rho(\mathbf{r})$, by

$$\phi(\mathbf{r}) = \int_V d^3r' G(\mathbf{r}, \mathbf{r}') \rho(\mathbf{r}') \quad (2.1.S.14)$$

When V is the entire universe, with the bounding surface $S \rightarrow \infty$, and all charge is localized (i.e. $\rho(\mathbf{r}) \rightarrow 0$ sufficiently fast as $|\mathbf{r}| \rightarrow \infty$) then $G(\mathbf{r}, \mathbf{r}')$ is just the familiar Coulomb potential of a point charge,

$$G(\mathbf{r}, \mathbf{r}') = \frac{1}{|\mathbf{r} - \mathbf{r}'|} \quad (2.1.S.15)$$

Here we want to discuss the Dirichlet problem where the system has a boundary S , and the value of ϕ is specified on S . What then is the appropriate Green's function $G_D(\mathbf{r}, \mathbf{r}')$?

Consider Green's 2nd identity with the integration variable being \mathbf{r}'

$$\int_V d^3r' (\phi \nabla'^2 \psi - \psi \nabla'^2 \phi) = \oint_S da' \left(\phi \frac{\partial \psi}{\partial n'} - \psi \frac{\partial \phi}{\partial n'} \right) \quad (2.1.S.16)$$

Apply this with $\phi(\mathbf{r}')$ being the electrostatic potential, so that $\nabla'^2 \phi(\mathbf{r}') = -4\pi\rho(\mathbf{r}')$, and $\psi(\mathbf{r}') = G(\mathbf{r}, \mathbf{r}')$ is the Green's function satisfying, $\nabla'^2 G(\mathbf{r}, \mathbf{r}') = -4\pi\delta(\mathbf{r} - \mathbf{r}')$.

We have seen that one solution to Poisson's equation is just $G(\mathbf{r}, \mathbf{r}') = 1/|\mathbf{r} - \mathbf{r}'|$. But a more general solution is

$$G(\mathbf{r}, \mathbf{r}') = \frac{1}{|\mathbf{r} - \mathbf{r}'|} + F(\mathbf{r}, \mathbf{r}') \quad (2.1.S.17)$$

where $\nabla'^2 F(\mathbf{r}, \mathbf{r}') = 0$ for all \mathbf{r}' in the volume V . Our goal is to choose $F(\mathbf{r}, \mathbf{r}')$ to simplify the solution of ϕ .

Substitute the above into Green's 2nd identity to get,

$$\int_V d^3r' (\phi(\mathbf{r}') \nabla'^2 G(\mathbf{r}, \mathbf{r}') - G(\mathbf{r}, \mathbf{r}') \nabla'^2 \phi(\mathbf{r}')) = \int_V d^3r' (\phi(\mathbf{r}') [-4\pi\delta(\mathbf{r} - \mathbf{r}')] - G(\mathbf{r}, \mathbf{r}') [-4\pi\rho(\mathbf{r}')]) \quad (2.1.S.18)$$

$$= -4\pi\phi(\mathbf{r}) + 4\pi \int_V d^3r' G(\mathbf{r}, \mathbf{r}') \rho(\mathbf{r}') = \oint_S da' \left(\phi \frac{\partial G}{\partial n'} - G \frac{\partial \phi}{\partial n'} \right) \quad \text{for } \mathbf{r} \text{ in the volume } V \quad (2.1.S.19)$$

We can rewrite this as

$$\phi(\mathbf{r}) = \int_V d^3r' G(\mathbf{r}, \mathbf{r}') \rho(\mathbf{r}') + \frac{1}{4\pi} \oint_S da' \left(G(\mathbf{r}, \mathbf{r}') \frac{\partial \phi(\mathbf{r}')}{\partial n'} - \phi(\mathbf{r}') \frac{\partial G(\mathbf{r}, \mathbf{r}')}{\partial n'} \right) \quad (2.1.S.20)$$

If we can choose $F(\mathbf{r}, \mathbf{r}')$ such that $G(\mathbf{r}, \mathbf{r}') = \frac{1}{|\mathbf{r} - \mathbf{r}'|} + F(\mathbf{r}, \mathbf{r}') = 0$ for any \mathbf{r}' on the bounding surface S , then the above simplifies to

$$\boxed{\phi(\mathbf{r}) = \int_V d^3r' G_D(\mathbf{r}, \mathbf{r}') \rho(\mathbf{r}') - \frac{1}{4\pi} \oint_S da' \phi(\mathbf{r}') \frac{\partial G_D(\mathbf{r}, \mathbf{r}')}{\partial n'}} \quad (2.1.S.21)$$

If we can find such an $F(\mathbf{r}, \mathbf{r}')$, then the Green's function so constructed is the Green's function for the Dirichlet boundary condition, hence we denote it G_D . Since one knows $\rho(\mathbf{r})$ for \mathbf{r} inside the volume V , and one knows the boundary condition specifying the value of $\phi(\mathbf{r})$ for \mathbf{r} on the surface S , then if one knows $G_D(\mathbf{r}, \mathbf{r}')$ one can in principle do all the integrations in Eq. (2.1.S.21) and so get the desired solution for $\phi(\mathbf{r})$.

Finding such an $G_D(\mathbf{r}, \mathbf{r}')$ is therefore equivalent to finding an $F(\mathbf{r}, \mathbf{r}')$ such that $\nabla'^2 F(\mathbf{r}, \mathbf{r}') = 0$ for all \mathbf{r}' in V (so F solves Laplace's equation) and $F(\mathbf{r}, \mathbf{r}') = -1/|\mathbf{r} - \mathbf{r}'|$ for \mathbf{r}' on the boundary surface S . By our previous uniqueness

demonstration, there always exists a unique solution for F with these properties (though it may not be easy to determine).

Green's Function for the Neumann Boundary Condition

Considering Eq. (2.1.S.20), and seeing how we dealt with the Dirichlet problem, one might think that one should try to find an $F(\mathbf{r}, \mathbf{r}')$ such that $\partial G(\mathbf{r}, \mathbf{r}')/\partial \mathbf{r}' = 0$ on the boundary surface S . But it turns out that this is not possible.

Consider

$$\int_V d^3 r' \nabla'^2 G(\mathbf{r}, \mathbf{r}') = \int_V d^3 r' \nabla' \cdot \nabla' G(\mathbf{r}, \mathbf{r}') = \oint_S da' \hat{\mathbf{n}} \cdot \nabla' G(\mathbf{r}, \mathbf{r}') = \oint_S da' \frac{\partial G(\mathbf{r}, \mathbf{r}')}{\partial n'} \quad (2.1.S.22)$$

But we know that

$$\nabla'^2 G(\mathbf{r}, \mathbf{r}') = -4\pi\delta(\mathbf{r} - \mathbf{r}') \quad \text{because } G(\mathbf{r}, \mathbf{r}') \text{ must solve Poisson's equation} \quad (2.1.S.23)$$

So for \mathbf{r} in V ,

$$\int_V d^3 r' \nabla'^2 G(\mathbf{r}, \mathbf{r}') = -4\pi = \oint_S da' \frac{\partial G(\mathbf{r}, \mathbf{r}')}{\partial n'} \quad (2.1.S.24)$$

So we cannot have a G such that $\partial G/\partial n' = 0$ for all \mathbf{r}' on S , because then the integral over the surface would vanish instead of equaling -4π .

So instead we make the next simplest choice. We want to find an $F(\mathbf{r}, \mathbf{r}')$ such that $G(\mathbf{r}, \mathbf{r}')$ obeys

$$\frac{\partial G(\mathbf{r}, \mathbf{r}')}{\partial n'} = \frac{-4\pi}{\mathcal{A}} \quad \text{for all } \mathbf{r}' \text{ on the surface } S. \text{ Here } \mathcal{A} \text{ is the area of the surface } S. \quad (2.1.S.25)$$

This gives the Neumann Green's function G_N . From Eq. (2.1.S.20) we have,

$$\phi(\mathbf{r}) = \int_V d^3 r' G_N(\mathbf{r}, \mathbf{r}') \rho(\mathbf{r}') + \frac{1}{4\pi} \oint_S da' G_N(\mathbf{r}, \mathbf{r}') \frac{\partial \phi(\mathbf{r}')}{\partial n'} - \frac{1}{4\pi} \oint_S da' \phi(\mathbf{r}') \left(\frac{-4\pi}{\mathcal{A}} \right) \quad (2.1.S.26)$$

which gives,

$$\boxed{\phi(\mathbf{r}) = \int_V d^3 r' G_N(\mathbf{r}, \mathbf{r}') \rho(\mathbf{r}') + \frac{1}{4\pi} \oint_S da' G_N(\mathbf{r}, \mathbf{r}') \frac{\partial \phi(\mathbf{r}')}{\partial n'}} + \langle \phi \rangle_S \quad (2.1.S.27)$$

where $\langle \phi \rangle_S$ is just the value of ϕ averaged over the surface S . But most importantly, $\langle \phi \rangle_S$ is just a constant, and so does not effect the electric field $\mathbf{E} = -\nabla\phi$ at all!

Since $\rho(\mathbf{r})$ is specified in the volume V , and $\partial\phi/\partial n$ is specified on the surface S , then the above gives the solution for $\phi(\mathbf{r})$ for all \mathbf{r} in V , within an additive constant that is of no physical consequence.

So determining $G_N(\mathbf{r}, \mathbf{r}')$ is equivalent to finding an $F(\mathbf{r}, \mathbf{r}')$ such that $\nabla'^2 F(\mathbf{r}, \mathbf{r}') = 0$ for \mathbf{r}' in V , and $\partial F(\mathbf{r}, \mathbf{r}')/\partial n' = -4\pi/\mathcal{A}$ for all \mathbf{r}' on S .

There always exists a unique (within an additive constant) solution to this problem.

While G_D and G_N always exist in principle, they depend in detail on the shape of the surface S and are difficult to find except for simple geometries.

Note, in the discussion in this section we have defined the Green's function by $\nabla'^2 G(\mathbf{r}, \mathbf{r}') = -4\pi\delta(\mathbf{r}, \mathbf{r}')$. But in our earlier discussion of the Green's function in the Notes 2-1 we had defined the Green's function by $\nabla^2 G(\mathbf{r}, \mathbf{r}') = -4\pi\delta(\mathbf{r} - \mathbf{r}')$. In the present section the derivatives are with respect to \mathbf{r}' , while in the earlier section the derivatives are with respect to \mathbf{r} . The equivalence of these two different definitions for G is obtained by noting that one can

prove the symmetry property $G(\mathbf{r}, \mathbf{r}') = G(\mathbf{r}', \mathbf{r})$ for the Dirichlet boundary condition, and one can impose it as an additional requirement for the Neumann boundary condition. We demonstrate this below.

We use the Green's 2nd identity, with $\phi(\mathbf{r}'') = G(\mathbf{r}, \mathbf{r}'')$, $\psi(\mathbf{r}'') = G(\mathbf{r}', \mathbf{r}'')$, and the integration variable as \mathbf{r}'' , to get,

$$\int_V d^3r'' [G(\mathbf{r}, \mathbf{r}'') \nabla''^2 G(\mathbf{r}', \mathbf{r}'') - G(\mathbf{r}', \mathbf{r}'') \nabla''^2 G(\mathbf{r}, \mathbf{r}'')] = \oint_S da'' \left[G(\mathbf{r}, \mathbf{r}'') \frac{\partial G(\mathbf{r}', \mathbf{r}'')}{\partial n''} - G(\mathbf{r}', \mathbf{r}'') \frac{\partial G(\mathbf{r}, \mathbf{r}'')}{\partial n''} \right] \quad (2.1.S.28)$$

Now use the definition of the Green's function, $\nabla'' G(\mathbf{r}, \mathbf{r}'') = -4\pi\delta(\mathbf{r} - \mathbf{r}'')$, to get,

$$-4\pi [G(\mathbf{r}, \mathbf{r}') - G(\mathbf{r}', \mathbf{r})] = \oint_S da'' \left[G(\mathbf{r}, \mathbf{r}'') \frac{\partial G(\mathbf{r}', \mathbf{r}'')}{\partial n''} - G(\mathbf{r}', \mathbf{r}'') \frac{\partial G(\mathbf{r}, \mathbf{r}'')}{\partial n''} \right] \quad (2.1.S.29)$$

For the Dirichlet boundary condition we know that $G_D(\mathbf{r}, \mathbf{r}'') = 0$ for \mathbf{r}'' on the surface S . Hence the surface integral on the right hand side vanishes and we have $G_D(\mathbf{r}, \mathbf{r}') = G_D(\mathbf{r}', \mathbf{r})$ is symmetric in $\mathbf{r} \leftrightarrow \mathbf{r}'$.

For the Neumann boundary condition we have that $\frac{\partial G_N(\mathbf{r}, \mathbf{r}'')}{\partial n''} = \frac{-4\pi}{\mathcal{A}}$ for \mathbf{r}'' on the surface S . So Eq. (2.1.S.29) becomes,

$$-4\pi [G_N(\mathbf{r}, \mathbf{r}') - G_N(\mathbf{r}', \mathbf{r})] = \oint_S da'' \left[G_N(\mathbf{r}, \mathbf{r}'') \left(\frac{-4\pi}{\mathcal{A}} \right) - G_N(\mathbf{r}', \mathbf{r}'') \left(\frac{-4\pi}{\mathcal{A}} \right) \right] \quad (2.1.S.30)$$

So now let us now construct,

$$\tilde{G}_N(\mathbf{r}, \mathbf{r}') = G_N(\mathbf{r}, \mathbf{r}') - \frac{1}{\mathcal{A}} \oint_S da'' G_N(\mathbf{r}, \mathbf{r}'') \quad (2.1.S.31)$$

From Eq. (2.1.S.30) we then conclude that $\tilde{G}_N(\mathbf{r}, \mathbf{r}') = \tilde{G}_N(\mathbf{r}', \mathbf{r})$ is symmetric in $\mathbf{r} \leftrightarrow \mathbf{r}'$. Moreover, $\tilde{G}_N(\mathbf{r}, \mathbf{r}')$ has all the desired properties of the original Neumann Green's function. Since the second term on the right hand side of Eq. (2.1.S.31) does not depend on \mathbf{r}' , it follows that $\nabla'^2 \tilde{G}_N(\mathbf{r}, \mathbf{r}') = \nabla'^2 G_N(\mathbf{r}, \mathbf{r}') = -4\pi\delta(\mathbf{r} - \mathbf{r}')$, and that $\partial \tilde{G}_N(\mathbf{r}, \mathbf{r}') / \partial n' = \partial G_N(\mathbf{r}, \mathbf{r}') / \partial n' = -4\pi / \mathcal{A}$. So we have constructed a Neumann Green's function $\tilde{G}(\mathbf{r}, \mathbf{r}')$ that has the desired symmetry.