Green functions: formal developments

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1 Green's Theorem

To develop a general method for solving the Poisson equation, we need a purely mathematical result: Green's theorem.

First, we establish a simple vector calculus identity,

$$\boldsymbol{\nabla}\cdot(f\boldsymbol{\nabla}g)=\boldsymbol{\nabla}f\cdot\boldsymbol{\nabla}g+f\boldsymbol{\nabla}^2 g$$

This relation is not hard to prove. We can just expand the del operator in Cartesian coordinates,

$$\boldsymbol{\nabla}=\hat{\mathbf{i}}\frac{\partial}{\partial x}+\hat{\mathbf{j}}\frac{\partial}{\partial y}+\hat{\mathbf{k}}\frac{\partial}{\partial z}$$

Substituting in the left hand side,

$$\begin{aligned}
\boldsymbol{\nabla}\cdot(f\boldsymbol{\nabla}g) &= \left(\hat{\mathbf{i}}\frac{\partial}{\partial x}+\hat{\mathbf{j}}\frac{\partial}{\partial y}+\hat{\mathbf{k}}\frac{\partial}{\partial z}\right)\cdot\left(f\left(\hat{\mathbf{i}}\frac{\partial g}{\partial x}+\hat{\mathbf{j}}\frac{\partial g}{\partial y}+\hat{\mathbf{k}}\frac{\partial g}{\partial z}\right)\right)\\
&= \hat{\mathbf{i}}\frac{\partial}{\partial x}\cdot\left(f\left(\hat{\mathbf{i}}\frac{\partial g}{\partial x}+\hat{\mathbf{j}}\frac{\partial g}{\partial y}+\hat{\mathbf{k}}\frac{\partial g}{\partial z}\right)\right)+\hat{\mathbf{j}}\frac{\partial}{\partial y}\cdot\left(f\left(\hat{\mathbf{i}}\frac{\partial g}{\partial x}+\hat{\mathbf{j}}\frac{\partial g}{\partial y}+\hat{\mathbf{k}}\frac{\partial g}{\partial z}\right)\right)\\
&\quad+\hat{\mathbf{k}}\frac{\partial}{\partial z}\cdot\left(f\left(\hat{\mathbf{i}}\frac{\partial g}{\partial x}+\hat{\mathbf{j}}\frac{\partial g}{\partial y}+\hat{\mathbf{k}}\frac{\partial g}{\partial z}\right)\right)
\end{aligned}$$

It is easiest to take the dot products first. Since $\hat{\mathbf{i}},\hat{\mathbf{j}},\hat{\mathbf{k}}$ are independent of position (unlike, say, $\hat{\boldsymbol{r}},\hat{\boldsymbol{\theta}},\hat{\boldsymbol{\phi}}$), we can bring them inside the derivative. Then we have

$$\begin{aligned}
\boldsymbol{\nabla}\cdot(f\boldsymbol{\nabla}g) &= \hat{\mathbf{i}}\frac{\partial}{\partial x}\cdot\left(f\left(\hat{\mathbf{i}}\frac{\partial g}{\partial x}+\hat{\mathbf{j}}\frac{\partial g}{\partial y}+\hat{\mathbf{k}}\frac{\partial g}{\partial z}\right)\right)+\hat{\mathbf{j}}\frac{\partial}{\partial y}\cdot\left(f\left(\hat{\mathbf{i}}\frac{\partial g}{\partial x}+\hat{\mathbf{j}}\frac{\partial g}{\partial y}+\hat{\mathbf{k}}\frac{\partial g}{\partial z}\right)\right)\\
&\quad+\hat{\mathbf{k}}\frac{\partial}{\partial z}\cdot\left(f\left(\hat{\mathbf{i}}\frac{\partial g}{\partial x}+\hat{\mathbf{j}}\frac{\partial g}{\partial y}+\hat{\mathbf{k}}\frac{\partial g}{\partial z}\right)\right)\\
&= \frac{\partial}{\partial x}\left(f\frac{\partial g}{\partial x}\right)+\frac{\partial}{\partial y}\left(f\frac{\partial g}{\partial y}\right)+\frac{\partial}{\partial z}\left(f\frac{\partial g}{\partial z}\right)\\
&= \left(\frac{\partial f}{\partial x}\frac{\partial g}{\partial x}+f\frac{\partial^2 g}{\partial x^2}\right)+\left(\frac{\partial f}{\partial y}\frac{\partial g}{\partial y}+f\frac{\partial^2 g}{\partial y^2}\right)+\left(\frac{\partial f}{\partial z}\frac{\partial g}{\partial z}+f\frac{\partial^2 g}{\partial z^2}\right)\\
&= \frac{\partial f}{\partial x}\frac{\partial g}{\partial x}+\frac{\partial f}{\partial y}\frac{\partial g}{\partial y}+\frac{\partial f}{\partial z}\frac{\partial g}{\partial z}+f\left(\frac{\partial^2 g}{\partial x^2}+\frac{\partial^2 g}{\partial y^2}+\frac{\partial^2 g}{\partial z^2}\right)\\
&= \frac{\partial f}{\partial x}\frac{\partial g}{\partial x}+\frac{\partial f}{\partial y}\frac{\partial g}{\partial y}+\frac{\partial f}{\partial z}\frac{\partial g}{\partial z}+f\left(\frac{\partial^2 g}{\partial x^2}+\frac{\partial^2 g}{\partial y^2}+\frac{\partial^2 g}{\partial z^2}\right)\\
&= \boldsymbol{\nabla}f\cdot\boldsymbol{\nabla}g+f\boldsymbol{\nabla}^2 g
\end{aligned}$$

Since the dot product, gradient and Laplacian are vector operators which are independent of coordinate system,

$$\boldsymbol{\nabla}\cdot(f\boldsymbol{\nabla}g)=\boldsymbol{\nabla}f\cdot\boldsymbol{\nabla}g+f\boldsymbol{\nabla}^2g$$

must now hold in any coordinates, not just Cartesian.

This calculation is shorter once you get used to index notation. If we set

$$\hat{\mathbf{e}}^i\equiv\left(\hat{\mathbf{i}},\hat{\mathbf{j}},\hat{\mathbf{k}}\right)$$

with $i=1,2,3$ telling us *which* basis vector we mean, not the components. Thus, for any orthonormal basis, we may write $\hat{\mathbf{e}}^i\cdot\hat{\mathbf{e}}^j=\delta^{ij}$. With this, we may write the gradient operator as a sum,

$$\boldsymbol{\nabla}=\sum_{i=1}^{3}\hat{\mathbf{e}}^i\frac{\partial}{\partial x^i}$$

This is even shorter with the Einstein summation convention: whenever we see a pair of indices, we assume there is a sum. Then we have, simply

$$\boldsymbol{\nabla}=\hat{\mathbf{e}}^i\frac{\partial}{\partial x^i}$$

We just have to be sure to use a different letter for a different sum. Finally, let the partial derivative be abbreviated to $\partial_i\equiv\frac{\partial}{\partial x^i}$, making the gradient just $\boldsymbol{\nabla}=\hat{\mathbf{e}}^i\partial_i$.

Now reconsider the calculation above:

$$\begin{aligned}\boldsymbol{\nabla}\cdot(f\boldsymbol{\nabla}g) &= \hat{\mathbf{e}}^i\partial_i\cdot\left(f\hat{\mathbf{e}}^k\partial_k g\right)\\ &= \hat{\mathbf{e}}^i\cdot\hat{\mathbf{e}}^k\partial_i\left(f\partial_k g\right)\\ &= \delta^{ik}\left(\partial_i f\partial_k g+f\partial_i\partial_k g\right)\\ &= \delta^{ik}\partial_i f\partial_k g+f\delta^{ik}\partial_i\partial_k g\\ &= \boldsymbol{\nabla}f\cdot\boldsymbol{\nabla}g+f\boldsymbol{\nabla}^2 g\end{aligned}$$

Compare these five lines to the first version. This is why you should learn index notation.

Now, to prove Green's first identity, we begin with the divergence theorem:

$$\int_V\boldsymbol{\nabla}\cdot\mathbf{A}\,d^3x=\oint_S\mathbf{A}\cdot\mathbf{n}\,d^2x$$

This holds for any vector field $\mathbf{A}$. Let the vector field $\mathbf{A}$ have the particular form

$$\mathbf{A}=f\boldsymbol{\nabla}g$$

where $f(\mathbf{x}),g(\mathbf{x})$ are any two functions of position. Substituting,

$$\begin{aligned}\int_V\boldsymbol{\nabla}\cdot\mathbf{A}\,d^3x &= \oint_S\mathbf{A}\cdot\mathbf{n}\,d^2x\\ \int_V\boldsymbol{\nabla}\cdot(f\boldsymbol{\nabla}g)\,d^3x &= \oint_S(f\boldsymbol{\nabla}g)\cdot\mathbf{n}\,d^2x\\ \int_V\left(\boldsymbol{\nabla}f\cdot\boldsymbol{\nabla}g+f\boldsymbol{\nabla}^2g\right)d^3x &= \oint_S(f\boldsymbol{\nabla}g)\cdot\mathbf{n}\,d^2x\end{aligned}$$

where we used the relation derived above. This is Green's first identity.

Suppose we pick some f and g. Then we know that

$$\int_V\left(\boldsymbol{\nabla}f\cdot\boldsymbol{\nabla}g+f\boldsymbol{\nabla}^2g\right)d^3x=\oint_S(f\boldsymbol{\nabla}g)\cdot\mathbf{n}\,d^2x$$

However, since f and g are arbitrary, we may also write

$$\int_V \left(\nabla g\cdot\nabla f + g\nabla^2 f\right)\, d^3x = \oint_S \left(g\nabla f\right)\cdot\mathbf{n}\, d^2x$$

for the same f and g. Taking the difference of these two expressions (and using the symmetry of the dot product $\nabla g\cdot\nabla f = \nabla f\cdot\nabla g$), we have

$$\int_V \left(f\nabla^2 g - g\nabla^2 f\right)\, d^3x = \oint_S \left(f\nabla g - g\nabla f\right)\cdot\mathbf{n}\, d^2x$$

Since $\mathbf{n}$ is the outward unit normal to the surface S bounding the volume V

$$\mathbf{n}\cdot\nabla g = \frac{\partial g}{\partial n}$$

is just the derivative of g normal to S. We can therefore simplify the notation a little,

$$\int_V \left(f\nabla^2 g - g\nabla^2 f\right)\, d^3x = \oint_S \left(f\frac{\partial g}{\partial n} - g\frac{\partial f}{\partial n}\right) d^2x$$

This is *Green's theorem.*

1.1 Example: Mean value theorem (Jackson 1.10)

As an example of the use of Green's theorem, we solve problem 1.10 from Jackson

Prove that

$$\Phi\left(\mathcal{P}\right) = \oint_{Sphere} \Phi\left(x\right) d^2x$$

in charge-free space, where the integral is over any sphere centered on the point $\mathcal{P}$.

Start wtih Green's theorem

$$\int_V \left(f\nabla^2 g - g\nabla^2 f\right) d^3x = \oint_S \left(f\frac{\partial g}{\partial n} - g\frac{\partial f}{\partial n}\right) d^2x$$

Choose $f = \Phi$ and $g = \frac{1}{r}$. Then

$$\int_V \left(\Phi\nabla^2\left(\frac{1}{r}\right) - \frac{1}{r}\nabla^2\Phi\right) d^3x = \oint_S \left(\Phi\frac{\partial}{\partial n}\frac{1}{r} - \frac{1}{r}\frac{\partial\Phi}{\partial n}\right) d^2x$$

Since we are in charge-free space we know that

$$\nabla^2\Phi = 0$$

and we also have

$$\nabla^2\left(\frac{1}{r}\right) = -4\pi\delta^3\left(r\right)$$

Substituting,

$$-4\pi\int_V \delta^3\left(r\right)\Phi d^3x = \oint_S \left(\Phi\frac{\partial}{\partial n}\frac{1}{r} - \frac{1}{r}\frac{\partial\Phi}{\partial n}\right) d^2x$$

Now, with the surface S a sphere centered on $r = 0$, we have

$$\frac{\partial}{\partial n}\frac{1}{r} = \hat{\mathbf{r}}\cdot\left(\hat{\mathbf{r}}\frac{\partial}{\partial r}\right)\frac{1}{r} = -\frac{1}{r^2}$$

Finally, the last term may be evaluated using Gauss's law:

$$\begin{aligned}
\oint_S \frac{1}{r}\frac{\partial \Phi}{\partial n} d^2x &= -\oint_S \frac{1}{r}\mathbf{E}\cdot\hat{\mathbf{r}} d^2x \\
&= -\frac{1}{R}\oint_S \mathbf{E}\cdot\hat{\mathbf{r}} d^2x \\
&= -\frac{Q_{tot}}{\epsilon_0 R} \\
&= 0
\end{aligned}$$

Putting this all together, and carrying out the integral over the delta function,

$$\begin{aligned}
-4\pi\int_V \delta^3(r)\,\Phi d^3x &= \oint_S \left(\Phi\frac{\partial}{\partial n}\frac{1}{r} - \frac{1}{r}\frac{\partial \Phi}{\partial n}\right) d^2x \\
-4\pi\Phi(0) &= \oint_S \left(-\frac{1}{r^2}\right)\Phi d^2x \\
\Phi(0) &= \frac{1}{4\pi r^2}\oint_S \Phi d^2x
\end{aligned}$$

The right hand side is the average of the potential over the sphere, and the left side is the potential at the center.

1.2 Example: Solution of the Laplace equation over all space

The solution to the Laplace equation in all space, with the potential vanishing at infinity follows from the mean value theorem. Let $\mathcal{P}$ be any point, and S_R a sphere of radius R around it. Then the value of Φ at $\mathcal{P}$is given by

$$\Phi(\mathcal{P}) = \frac{1}{4\pi R^2}\oint_S \Phi(x)\, d^2x$$

where the integral is over the surface of the sphere. Taking the limit as $R \to \infty$ and using $\Phi(\infty) = 0$,

$$\begin{aligned}
\Phi(\mathcal{P}) &= \lim_{R\to\infty}\left[\frac{1}{4\pi R^2}\oint_S \Phi(x)\, d^2x\right] \\
&= \lim_{R\to\infty}\left[\frac{1}{4\pi R^2}\oint_S \Phi(\infty)\, d^2x\right] \\
&= \lim_{R\to\infty}\left[\Phi(\infty)\cdot\frac{1}{4\pi R^2}\oint_S d^2x\right] \\
&= \lim_{R\to\infty}[0\cdot 1] \\
&= 0
\end{aligned}$$

Since $\mathcal{P}$ is arbitrary, $\Phi(\mathbf{x}) = 0$. The unique solution to the Laplace equation over all space, with Φ vanishing at infinity, is zero.

1.3 The absence of local extrema

The mean value theorem holds for *any* sphere surrounding any point. Now suppose there is a local maximum (or minimum) of Φ at some point $\mathcal{P}_0$. Then by continuity of Φ, there is a neighborhood of $\mathcal{P}_0$ on which $\Phi(\mathbf{x}) < \Phi(\mathcal{P}_0)$. Choose a sphere contained entirely within this neighborhood. The average of Φ over this sphere must equal $\Phi(\mathcal{P}_0)$, but this is impossible since all values of $\Phi(S)$ are less than $\Phi(\mathcal{P}_0)$. This is a contradition, so there cannot be any local maximum or minimum of Φ within the entire region. This means that Φ takes all of its maximum and minimum values on the boundary of the region.

1.4 Uniqueness of solutions to the Laplace equation with given boundary conditions

Now suppose we have the Laplace equation for a region V with specified boundary conditions $\Phi(S)$ on the boundary surface S of V, possibly with multiple pieces. We prove uniqueness of the solution by finding a contradiction. Assume that f and g both satisfy the Laplace equation,

$$\begin{aligned}\nabla^2 f &= 0\\ \nabla^2 g &= 0\end{aligned}$$

with the same boundary conditions,

$$f(S) = g(S) = \Phi(S)$$

Then the function $h \equiv f - g$ also satisfies the Laplace equation with boundary values $h(S) = 0$. But by the absence of maxima or minima within S, $h(S) = 0$ must be both the maximum and the minimum value of h everywhere in the region. Therefore, $h(\mathbf{x}) = 0$ throughout V and we have $f = g$.

Therefore, solutions of the Laplace equation with given boundary conditions are unique.

2 Formal solution of the Poisson equation

We now use Green's theorem and the ideas of the previous Notes to write a complete formal solution to the Poisson equation, satisfying given boundary conditions.

Suppose we can find a function, $G(\mathbf{x}, \mathbf{x}')$ satisfying

$$\nabla^2 G(\mathbf{x}, \mathbf{x}') = -4\pi\delta^3(\mathbf{x} - \mathbf{x}') \tag{1}$$

and satisfying the given boundary conditions, where the Laplacian is with respect to the unprimed coordinates. The *Green function*, $G(\mathbf{x}, \mathbf{x}')$, is the solution of the Poisson equation for a unit point charge $\frac{q}{\epsilon_0} = 1$ at $\mathbf{x}'$. It is continuous in both $\mathbf{x}$ and $\mathbf{x}'$, and symmetric, $G(\mathbf{x}, \mathbf{x}') = G(\mathbf{x}', \mathbf{x})$.

The simplest example of a Green function is for an *isolated* point charge, with the potential vanishing at infinity. We have already shown that

$$\nabla^2 \frac{1}{|\mathbf{x} - \mathbf{x}'|} = -4\pi\delta^3(\mathbf{x} - \mathbf{x}')$$

we immediately have

$$G(\mathbf{x}, \mathbf{x}') = \frac{1}{|\mathbf{x} - \mathbf{x}'|} + F(\mathbf{x})$$

where F satisfies the Laplace equation, $\nabla^2 F = 0$. By uniqueness, the function F must be determined by the boundary conditions. In the present case, we ask for $G(\mathbf{x}, \mathbf{x}')$ to vanish at $\mathbf{x} \to \infty$. Since the first term in $G(\mathbf{x}, \mathbf{x}')$ already satisfies this, we require the same condition for F:

$$\begin{aligned}\nabla^2 F &= 0\\ F(\infty) &= 0\end{aligned}$$

The arguments of the preceeding section show that $F(\mathbf{x}) = 0$ is the unique solution to this, so the Green function for an isolated point charge is $G(\mathbf{x}, \mathbf{x}') = \frac{1}{|\mathbf{x} - \mathbf{x}'|}$.

As described in a preceding Note, If we have a localized distribution of charge, $\rho(\mathbf{x}')$, in empty space, the potential vanishes at infinity and we can use this Green function to find the potential everywhere by superposition. Each infinitesimal charge

$$\frac{1}{\epsilon_0} dq = \frac{1}{\epsilon_0} \rho(\mathbf{x}') \, d^3x'$$

gives a contribution to the potential of $d\Phi(\mathbf{x}) = \frac{1}{4\pi\epsilon_0}\frac{1}{|\mathbf{x}-\mathbf{x}'|}\rho(\mathbf{x}')\,d^3x'$, so integrating,

$$\Phi(\mathbf{x}) = \frac{1}{\epsilon_0}\int \frac{\rho(\mathbf{x}')}{|\mathbf{x}-\mathbf{x}'|}d^3x'$$

The procedure is idential for more general Green functions. Given $G(\mathbf{x},\mathbf{x}')$ satisfying eq.(1) and the given boundary conditions, a full solution is found by taking a superposition. Thus, setting

$$\Phi(\mathbf{x}) = \frac{1}{4\pi\varepsilon_0}\int G(\mathbf{x},\mathbf{x}')\,\rho(\mathbf{x}')\,d^3x'$$

we see that

$$\begin{aligned}
\nabla^2\Phi(\mathbf{x}) &= \frac{1}{4\pi\epsilon_0}\nabla^2\int G(\mathbf{x},\mathbf{x}')\,\rho(\mathbf{x}')\,d^3x' \\
&= \frac{1}{4\pi\epsilon_0}\int\left(\nabla^2 G(\mathbf{x},\mathbf{x}')\right)\rho(\mathbf{x}')\,d^3x' \\
&= -\frac{1}{\epsilon_0}\int\delta^3(\mathbf{x}-\mathbf{x}')\,\rho(\mathbf{x}')\,d^3x' \\
&= -\frac{1}{\epsilon_0}\rho(\mathbf{x})
\end{aligned}$$

and we have a solution.

2.1 The existence of general solutions

Now we turn to a careful consideration of the b

The freedom to choose $F(\mathbf{x})$ allows us to solve with more general boundary conditions. Suppose our problem requires solutions with values $\Phi(S)$ on an arbitrary closed boundary surface S. Then using Green's theorem

$$\int_V\left(f\boldsymbol{\nabla}^2 g - g\boldsymbol{\nabla}^2 f\right)\,d^3x' = \oint_S\left(f\frac{\partial g}{\partial n'} - g\frac{\partial f}{\partial n'}\right)\,d^2x'$$

with

$$\begin{aligned}
f &= \Phi(\mathbf{x}') \\
g &= G(\mathbf{x},\mathbf{x}')
\end{aligned}$$

where

$$\begin{aligned}
\boldsymbol{\nabla}^2\Phi(\mathbf{x}) &= -\frac{\rho(\mathbf{x})}{\epsilon_0} \\
\left(\boldsymbol{\nabla}'\right)^2 G(\mathbf{x},\mathbf{x}') &= -4\pi\delta^3(\mathbf{x}-\mathbf{x}')
\end{aligned}$$

we find

$$\begin{aligned}
\int_V\left(\Phi(\mathbf{x}')\,\boldsymbol{\nabla}^2 G(\mathbf{x},\mathbf{x}') - G(\mathbf{x},\mathbf{x}')\,\boldsymbol{\nabla}^2\Phi(\mathbf{x}')\right)\,d^3x &= \oint_S\left(\Phi(\mathbf{x}')\frac{\partial G(\mathbf{x},\mathbf{x}')}{\partial n} - G(\mathbf{x},\mathbf{x}')\frac{\partial\Phi(\mathbf{x}')}{\partial n}\right)\,d^2x \\
\int_V\left(-4\pi\Phi(\mathbf{x}')\,\delta^3(\mathbf{x}-\mathbf{x}') + G(\mathbf{x},\mathbf{x}')\frac{\rho(\mathbf{x}')}{\epsilon_0}\right)\,d^3x' &= \oint_S\left(\Phi(\mathbf{x}')\frac{\partial G(\mathbf{x},\mathbf{x}')}{\partial n'} - G(\mathbf{x},\mathbf{x}')\frac{\partial\Phi(\mathbf{x}')}{\partial n'}\right)\,d^2x' \\
-4\pi\Phi(\mathbf{x}) + \frac{1}{\epsilon_0}\int_V G(\mathbf{x},\mathbf{x}')\,\rho(\mathbf{x}')\,d^3x' &= \oint_S\left(\Phi(\mathbf{x}')\frac{\partial G(\mathbf{x},\mathbf{x}')}{\partial n'} - G(\mathbf{x},\mathbf{x}')\frac{\partial\Phi(\mathbf{x}')}{\partial n'}\right)\,d^2x'
\end{aligned}$$

Solving for the potential we have

$$\Phi(\mathbf{x}) = \frac{1}{4\pi\epsilon_0}\int_V G(\mathbf{x},\mathbf{x}')\,\rho(\mathbf{x}')\;d^3x' - \oint_S \left(\Phi(\mathbf{x}')\frac{\partial G(\mathbf{x},\mathbf{x}')}{\partial n'} - G(\mathbf{x},\mathbf{x}')\frac{\partial \Phi(\mathbf{x}')}{\partial n'}\right) d^2x'$$

As we show below, we cannot specify both $G(\mathbf{x},\mathbf{x}')$ and its normal derivative $\frac{\partial G(\mathbf{x},\mathbf{x}')}{\partial n'}$ on the boundary. One or the other of these is sufficient to uniquely determine $G(\mathbf{x},\mathbf{x}')$. Therefore, we get two extreme cases, called Dirichlet and Neuman boundary conditions. Combinations are also possible.

2.1.1 Dirichlet boundary conditions

For the case of *Dirichlet boundary conditions*, we require

$$G(\mathbf{x},\mathbf{x}')|_{\mathbf{x}'\in S} = 0$$

This uniquely specifies $G(\mathbf{x},\mathbf{x}')$ within S, and gives the solution

$$\Phi(\mathbf{x}) = \frac{1}{4\pi\epsilon_0}\int_V G(\mathbf{x},\mathbf{x}')\,\rho(\mathbf{x}')\;d^3x' - \frac{1}{4\pi}\oint_S \Phi(\mathbf{x}')\frac{\partial G(\mathbf{x},\mathbf{x}')}{\partial n'}\,d^2x' \tag{2}$$

Noting that we know both $G(\mathbf{x},\mathbf{x}')$ and $\Phi(S)$, this gives the potential everywhere in the volume V.

To see that we have satisfied the boundary conditions, let $\mathbf{x}$ lie on S,

$$\begin{aligned}\Phi(\mathbf{x})|_{\mathbf{x}\in S} &= \frac{1}{4\pi\epsilon_0}\int_V G(\mathbf{x}|_S,\mathbf{x}')\,\rho(\mathbf{x}')\;d^3x' - \frac{1}{4\pi}\left[\oint_S \Phi(\mathbf{x}')\frac{\partial G(\mathbf{x},\mathbf{x}')}{\partial n'}\,d^2x'\right]_{\mathbf{x}\in S}\\ &= -\frac{1}{4\pi}\left[\oint_S \Phi(\mathbf{x}')\frac{\partial G(\mathbf{x},\mathbf{x}')}{\partial n'}\,d^2x'\right]_{\mathbf{x}\in S}\end{aligned}$$

To find the derivative of G, we integrate eq.(1) across the boundary,

$$\begin{aligned}\int \boldsymbol{\nabla}^2 G(\mathbf{x},\mathbf{x}')\,dn' &= -4\pi\int \delta^3(\mathbf{x}-\mathbf{x}')\,dn'\\ \int \boldsymbol{\nabla}\cdot\boldsymbol{\nabla} G(\mathbf{x},\mathbf{x}')\,dn' &= -4\pi\delta^2(\mathbf{x}-\mathbf{x}')\end{aligned}$$

Now, since $G(\mathbf{x},\mathbf{x}')$ is constant on S, $\nabla G(\mathbf{x},\mathbf{x}')$ is in the normal direction so the first integral is

$$\begin{aligned}\int \boldsymbol{\nabla}\cdot\boldsymbol{\nabla} G(\mathbf{x},\mathbf{x}')\,dn' &= \int \frac{\partial^2 G}{\partial n'^2}(\mathbf{x},\mathbf{x}')\,dn'\\ &= \frac{\partial G}{\partial n'}(\mathbf{x},\mathbf{x}')\end{aligned}$$

and we have

$$\frac{\partial G}{\partial n'}(\mathbf{x},\mathbf{x}') = -4\pi\delta^2(\mathbf{x}-\mathbf{x}')$$

Substituting into our expression for the potential,

$$\begin{aligned}\Phi(\mathbf{x})|_{\mathbf{x}\in S} &= -\frac{1}{4\pi}\left[\oint_S \Phi(\mathbf{x}')\frac{\partial G(\mathbf{x},\mathbf{x}')}{\partial n'}\,d^2x'\right]_{\mathbf{x}\in S}\\ &= \left[\oint_S \Phi(\mathbf{x}')\,\delta^2(\mathbf{x}-\mathbf{x}')\;d^2x'\right]_{\mathbf{x}\in S}\\ &= \Phi(\mathbf{x})|_{\mathbf{x}\in S}\end{aligned}$$

and the boundary condition is satisfied.

2.1.2 Neumann boundary conditions

For Neumann boundary conditions, we require a condition on the derivative, $\frac{\partial G}{\partial n'}(\mathbf{x},\mathbf{x}')$. If we integrate eq.(1) over our volume and use the divergence theorem,

$$\begin{aligned}
\int \boldsymbol{\nabla}^2 G(\mathbf{x},\mathbf{x}')\,d^3x' &= -4\pi \int \delta^3(\mathbf{x}-\mathbf{x}')\,d^3x' \\
\int \boldsymbol{\nabla}\cdot\boldsymbol{\nabla} G(\mathbf{x},\mathbf{x}')\,d^3x' &= -4\pi \\
\int \hat{\mathbf{n}}\cdot\boldsymbol{\nabla} G(\mathbf{x},\mathbf{x}')\,d^3x' &= -4\pi
\end{aligned}$$

so that the integral of the derivative over the boundary cannot vanish,

$$\oint_S \frac{\partial G(\mathbf{x},\mathbf{x}')}{\partial n'}\,d^2x' = -4\pi$$

Therefore, instead of choosing $\frac{\partial G}{\partial n'}$ to vanish on the boundary, we choose it constant

$$\left.\frac{\partial G}{\partial n'}(\mathbf{x},\mathbf{x}')\right|_{\mathbf{x}\in S} = -\frac{4\pi}{S}$$

where S is the area of the boundary. This is sufficient to uniquely determine G.

With the derivative fixed as the boundary condition, the potential is given by

$$\Phi(\mathbf{x}) = \frac{1}{4\pi\epsilon_0}\int_V G(\mathbf{x},\mathbf{x}')\,\rho(\mathbf{x}')\,d^3x' + \oint_S G(\mathbf{x},\mathbf{x}')\,\frac{\partial\Phi(\mathbf{x}')}{\partial n'}\,d^2x' + \frac{4\pi}{S}\oint_S \Phi(\mathbf{x}')\,d^2x' \tag{3}$$

where the additional term is just the average of the potential over the boundary. All terms on the right are now specified and we have found a solution for the potential.

3 Uniqueness of solutions to the Poisson equation

We now want to establish the uniqueness of solutions to our electrostatic problems,

$$\nabla^2\Phi = \frac{\rho}{\epsilon_0}$$

for a fixed source distribution, $\rho(\mathbf{x})$, and satisfying specified boundary conditions $\Phi(\mathbf{x})|_{\mathbf{x}\in S}$. However, we know that for any $\Phi(\mathbf{x})$ satisfying this equation, we may add a solution, $\Phi'(\mathbf{x})$, of the homogeneous (Laplace) equation,

$$\nabla^2\Phi'(\mathbf{x}) = 0$$

We complete a proof by showing that two solutions satisfying the same boundary conditions must be the same.

Suppose we have two solutions, Φ_1, Φ_2, satisfying the Poisson equation on V, and satisfying some specific condition on the boundary S. The boundary condition may be either the value of the potential on S or the value of the normal derivative, $\frac{\partial\Phi}{\partial n}$, on S. In either case, the difference of the two potentials,

$$U = \Phi_2 - \Phi_1$$

must satisfy the Laplace equation since

$$\begin{aligned}
\boldsymbol{\nabla}^2 U &= \boldsymbol{\nabla}^2(\Phi_2-\Phi_1) \\
&= \boldsymbol{\nabla}^2\Phi_2 - \boldsymbol{\nabla}^2\Phi_1 \\
&= \frac{1}{\epsilon_0}\rho - \frac{1}{\epsilon_0}\rho \\
&= 0
\end{aligned}$$

and similarly, will have vanishing boundary values, i.e., either

$$U(\mathbf{x})|_{x\in S} = 0$$

or

$$\left.\frac{\partial U(\mathbf{x})}{\partial n}\right|_{x\in S} = 0$$

Now use Green's first identity with $f = g = U$:

$$\begin{aligned}\int_V \left(\boldsymbol{\nabla} f\cdot\boldsymbol{\nabla} g + f\boldsymbol{\nabla}^2 g\right) d^3x &= \oint_S f\frac{\partial g}{\partial n} n\, d^2x \\ \int_V \left(\boldsymbol{\nabla} U\cdot\boldsymbol{\nabla} U + U\boldsymbol{\nabla}^2 U\right) d^3x &= \oint_S U\frac{\partial U}{\partial n}\, d^2x\end{aligned}$$

The boundary condition for U makes the right side vanish, which together with $\boldsymbol{\nabla}^2 U = 0$ reduces the identity to

$$\int_V \left(\boldsymbol{\nabla} U\cdot\boldsymbol{\nabla} U\right) d^3x = \int_V |\boldsymbol{\nabla} U|^2\, d^3x = 0$$

This implies $\boldsymbol{\nabla} U = 0$, so that $U = c$. Only the value of this constant remains unspecified, and the field, $E = -\boldsymbol{\nabla}\Phi$ is unique.

Since the theorem applies to U itself, U is uniquely determined by either $U = 0$ (Dirichlet boundary conditions) or $\frac{\partial U}{\partial n} = 0$ (Neumann boundary conditions) on the boundary. It would overspecify the solution to try to impose conditions on both U and its derivative. It is possible, however, to specify $U = 0$ on one part of S, and $\frac{\partial U}{\partial n} = 0$ on the remaining part, as long as the right side vanishes. The same applies to the Green function.

We conclude that specifying the Poisson equation for the potential together with Dirichlet or Neumann boundary conditions, determines the electic field uniquely.

4 Green function with spherical boundary conditions

To solve the Poisson equation with values of Φ specified on a sphere of radius a, we need a Green function satisfying

$$\begin{aligned}\boldsymbol{\nabla}^2 G(\mathbf{x},\mathbf{x}') &= -4\pi\delta^3(\mathbf{x}-\mathbf{x}') \\ G(\mathbf{x},\mathbf{x}')|_{r=a} &= 0\end{aligned}$$

and we would like the result to be expressed in terms of spherical coordinates. The second boundary may be taken either at the origin or infinity. For concreteness we look at the exterior case. The interior case is similar.

To begin, we note the solution for a single point charge q outside a grounded sphere at position $\mathbf{x}'$ is given by the image method as

$$\Phi(\mathbf{x}) = \frac{q}{4\pi\epsilon_0}\left(\frac{1}{|\mathbf{x}-\mathbf{x}'|} - \frac{a/r'}{\left|\mathbf{x}-\left(\frac{a}{r'}\right)^2\mathbf{x}'\right|}\right)$$

This satisfies

$$\boldsymbol{\nabla}^2\Phi(\mathbf{x}) = -\frac{1}{\epsilon_0} q\delta^3(\mathbf{x}-\mathbf{x}')$$

so that rescaling,

$$\boldsymbol{\nabla}^2\left(\frac{1}{|\mathbf{x}-\mathbf{x}'|} - \frac{a/r'}{\left|\mathbf{x}-\left(\frac{a}{r'}\right)^2\mathbf{x}'\right|}\right) = -4\pi\delta^3(\mathbf{x}-\mathbf{x}')$$

and we have the Green function.

Now, to express this in spherical coordinates,

$$\begin{aligned}\mathbf{x} &= (r,\theta,\varphi)\\ \mathbf{x}' &= (r',\theta',\varphi')\end{aligned}$$

we use the expansion in spherical harmonics,

$$\frac{1}{|\mathbf{x}-\mathbf{x}'|}=\sum_{l=0}^{\infty}\sum_{m=-l}^{l}\frac{4\pi}{2l+1}\frac{r_<^l}{r_>^{l+1}}Y_{lm}^*(\theta',\varphi')Y_{lm}(\theta,\varphi)$$

For the image charge we have $\frac{a^2}{r'^2}r' < r$, so

$$\begin{aligned}\frac{a/r'}{\left|\mathbf{x}-\left(\frac{a}{r'}\right)^2\mathbf{x}'\right|} &= \frac{a}{r'}\sum_{l=0}^{\infty}\sum_{m=-l}^{l}\frac{4\pi}{2l+1}\frac{\left(\frac{a^2}{r'}\right)^l}{r^{l+1}}Y_{lm}^*(\theta',\varphi')Y_{lm}(\theta,\varphi)\\ &= \sum_{l=0}^{\infty}\sum_{m=-l}^{l}\frac{4\pi}{2l+1}\frac{a^{2l+1}}{r^{l+1}r'^{l+1}}Y_{lm}^*(\theta',\varphi')Y_{lm}(\theta,\varphi)\end{aligned}$$

Substituting, we have the Green function for boundary conditions on a sphere and at infinity:

$$G(\mathbf{x},\mathbf{x}')=\sum_{l=0}^{\infty}\sum_{m=-l}^{l}\frac{4\pi}{2l+1}\left(\frac{r_<^l}{r_>^{l+1}}-\frac{a^{2l+1}}{r^{l+1}r'^{l+1}}\right)Y_{lm}^*(\theta',\varphi')Y_{lm}(\theta,\varphi)$$

Now, so solve

$$\begin{aligned}\boldsymbol{\nabla}^2\Phi(\mathbf{x}) &= -\frac{1}{\epsilon_0}\rho(\mathbf{x})\\ \Phi_S(\mathbf{x}) &= f(\theta,\varphi)\end{aligned}$$

we use our general solution,

$$\Phi(\mathbf{x}) = \frac{1}{4\pi\epsilon_0}\int_V G(\mathbf{x},\mathbf{x}')\rho(\mathbf{x}')\,d^3x' - \frac{1}{4\pi}\int_0^{\pi}\int_0^{2\pi} f(\theta',\varphi')\left[-\frac{\partial G(r,\theta,\varphi;a,\theta',\varphi')}{\partial r'}\right]a^2\sin\theta' d\theta' d\varphi'$$

The minus sign in the derivative of the Green fucntion is because we need the outward normal from the (exterior) region of interest. Because on the boundary sphere, $r'=a<r$, this derivative has the form

$$\begin{aligned}\frac{\partial G(r,\theta,\varphi;a,\theta',\varphi')}{\partial r'} &= \left[\frac{\partial}{\partial r'}\sum_{l=0}^{\infty}\sum_{m=-l}^{l}\frac{4\pi}{2l+1}\left(\frac{r_<^l}{r_>^{l+1}}-\frac{a^{2l+1}}{r^{l+1}r'^{l+1}}\right)Y_{lm}^*(\theta',\varphi')Y_{lm}(\theta,\varphi)\right]_{r'=a}\\ &= \left[\sum_{l=0}^{\infty}\sum_{m=-l}^{l}\frac{4\pi}{2l+1}\frac{\partial}{\partial r'}\left(\frac{r'^l}{r^{l+1}}-\frac{a^{2l+1}}{r^{l+1}r'^{l+1}}\right)Y_{lm}^*(\theta',\varphi')Y_{lm}(\theta,\varphi)\right]_{r'=a}\\ &= \sum_{l=0}^{\infty}\sum_{m=-l}^{l}\frac{4\pi}{2l+1}\left(\frac{la^{l-1}}{r^{l+1}}+\frac{(l+1)a^{2l+1}}{r^{l+1}a^{l+2}}\right)Y_{lm}^*(\theta',\varphi')Y_{lm}(\theta,\varphi)\\ &= 4\pi\sum_{l=0}^{\infty}\sum_{m=-l}^{l}\frac{a^{l-1}}{r^{l+1}}Y_{lm}^*(\theta',\varphi')Y_{lm}(\theta,\varphi)\end{aligned}$$

4.1 Example

Let the charge density vanish and the potential at $r = a$ be given by

$$\Phi_S(\mathbf{x}) = A\cos\theta$$

Then the potential exterior to $r = a$ is given by

$$\begin{aligned}
\Phi(\mathbf{x}) &= -\frac{A}{4\pi}\int_0^{\pi}\int_0^{2\pi}\cos\theta'\left[-4\pi\sum_{l=0}^{\infty}\sum_{m=-l}^{l}\frac{a^{l-1}}{r^{l+1}}Y_{lm}^*(\theta',\varphi')\,Y_{lm}(\theta,\varphi)\right]a^2\sin\theta' d\theta' d\varphi' \\
&= A\sum_{l=0}^{\infty}\sum_{m=-l}^{l}\frac{a^{l-1}}{r^{l+1}}Y_{lm}(\theta,\varphi)\int_0^{\pi}\int_0^{2\pi}Y_{lm}^*(\theta',\varphi')\cos\theta'\,a^2\sin\theta' d\theta' d\varphi'
\end{aligned}$$

To evaluate the integrals, we rewrite $\cos\theta'$ in terms of spherical harmonics,

$$\cos\theta' = \sqrt{\frac{4\pi}{3}}Y_{10}(\theta',\varphi')$$

Then

$$\begin{aligned}
\int_0^{\pi}\int_0^{2\pi}Y_{lm}^*(\theta',\varphi')\cos\theta'\,a^2\sin\theta' d\theta' d\varphi' &= \sqrt{\frac{4\pi}{3}}\int_0^{\pi}\int_0^{2\pi}Y_{lm}^*(\theta',\varphi')\,Y_{10}(\theta',\varphi')\;a^2\sin\theta' d\theta' d\varphi' \\
&= \sqrt{\frac{4\pi}{3}}\delta_{l1}\delta_{m0}
\end{aligned}$$

and we have

$$\begin{aligned}
\Phi(\mathbf{x}) &= A\sum_{l=0}^{\infty}\sum_{m=-l}^{l}\frac{a^{l-1}}{r^{l+1}}Y_{lm}(\theta,\varphi)\sqrt{\frac{4\pi}{3}}\delta_{l1}\delta_{m0}a^2 \\
&= \frac{Aa^2}{r^2}\cos\theta
\end{aligned}$$

which clearly satisfies the required boundary conditions at $r = a$ and infinity.