The Laplacian of the inverse distance and the Green function

1. The Poisson Equation

Consider the laws of electrostatics in cgs units,

$$\vec{\nabla}\cdot\vec{E} = 4\pi\rho\,, \qquad \vec{\nabla}\times\vec{E} = 0\,, \tag{1}$$

where $\vec{E}$ is the electric field vector and ρ is the local charge density. Since $\vec{\nabla}\times\vec{E} = 0$, it follows that $\vec{E}$ can be expressed as the gradient of a scalar function. Thus, we define the electric potential as

$$\vec{E} = -\boldsymbol{\nabla}\Phi\,. \tag{2}$$

Note that $\vec{\nabla}\times\vec{E} = -\vec{\nabla}\times\vec{\nabla}\Phi = 0$, since the curl of the gradient of any well-behaved scalar function is zero. Combining eqs. (1) and (2) yields

$$\vec{\nabla}\cdot\vec{E} = -\vec{\nabla}\cdot\boldsymbol{\nabla}\Phi = -\vec{\nabla}^{\mathbf{2}}\Phi = 4\pi\rho\,.$$

That is,

$$\vec{\nabla}^{\mathbf{2}}\Phi = -4\pi\rho\,. \tag{3}$$

This is the Poisson equation (or the inhomogeneous Laplace equation).

Consider a point charge located at the position $\vec{r}_{\mathbf{0}}$. Then, we can write

$$\rho(\vec{r}) = q\delta^3(\vec{r}-\vec{r}_{\mathbf{0}})\,.$$

The delta function representation of a point charge indicates that no charge exists anywhere other than at the position $\vec{r}_{\mathbf{0}}$. Moreover, the total charge contained in the point charge is

$$\int_V \rho(\vec{r})d^3r = q\int_V \delta^3(\vec{r}-\vec{r}_{\mathbf{0}}) = q\,, \tag{4}$$

where d^3r is the infinitesimal three-dimensional volume element and V is any finite volume that contains the point $\vec{r}_{\mathbf{0}}$.

Given a point charge located at the position $\vec{r}_{\mathbf{0}}$, the corresponding electric field is given by Coulomb's law (in cgs units),

$$\vec{E}(\vec{r}) = \frac{q(\vec{r}-\vec{r}_{\mathbf{0}})}{|\vec{r}-\vec{r}_{\mathbf{0}}|^3} = -q\vec{\nabla}\left(\frac{1}{|\vec{r}-\vec{r}_{\mathbf{0}}|}\right)\,.$$

From this, we can obtain the potential from eq. (2),

$$\Phi(\vec{r}) = \frac{q}{|\vec{r}-\vec{r}_{\mathbf{0}}|}\,.$$

2. The Laplacian of the inverse distance

The inverse distance between the vectors $\vec{\boldsymbol{r}}$ and $\vec{\boldsymbol{r}}_{\boldsymbol{0}}$ is given by the function,

$$d(\vec{\boldsymbol{r}}) = \frac{1}{|\vec{\boldsymbol{r}} - \vec{\boldsymbol{r}}_{\boldsymbol{0}}|}\,.$$

Here, $\vec{\boldsymbol{r}}_{\boldsymbol{0}}$ is a fixed location (such as the position of a point charge) and $\vec{\boldsymbol{r}}$ is the location of the observer. We shall compute the Laplacian of the inverse distance

$$\vec{\boldsymbol{\nabla}}^{\boldsymbol{2}} d(\vec{\boldsymbol{r}}) = \vec{\boldsymbol{\nabla}}^{\boldsymbol{2}}\left(\frac{1}{|\vec{\boldsymbol{r}} - \vec{\boldsymbol{r}}_{\boldsymbol{0}}|}\right)\,,$$

where $\vec{\boldsymbol{\nabla}}^{\boldsymbol{2}}$ involves derivatives with respect to $\vec{\boldsymbol{r}}$, with $\vec{\boldsymbol{r}}_{\boldsymbol{0}}$ held fixed. It is convenient to define a new variable $\vec{\boldsymbol{R}} \equiv \vec{\boldsymbol{r}} - \vec{\boldsymbol{r}}_{\boldsymbol{0}}$. Then, it follows that $\vec{\boldsymbol{\nabla}}^{\boldsymbol{2}}_{\boldsymbol{R}} = \vec{\boldsymbol{\nabla}}^{\boldsymbol{2}}_{\boldsymbol{r}}$, where the subscript indicates the variable employed by the corresponding derivatives.[1] Thus, we evaluate

$$\vec{\boldsymbol{\nabla}}^{\boldsymbol{2}}\left(\frac{1}{R}\right) = \frac{1}{R^2}\frac{\partial}{\partial R}\left\{R^2\frac{\partial}{\partial R}\left(\frac{1}{R}\right)\right\} = \frac{1}{R^2}\frac{\partial}{\partial R}(-1) = 0\,,$$

where we have performed the computation in spherical coordinates, where

$$\vec{\boldsymbol{\nabla}}^{\boldsymbol{2}}_{\boldsymbol{R}} = \frac{1}{R^2}\frac{\partial}{\partial R}\left(R^2\frac{\partial}{\partial R}\right) + \frac{1}{R^2\sin^2\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{R^2\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\,.$$

Of course, the angular derivatives vanish when applied to a radial function. Thus, we have apparently derived the result,

$$\vec{\boldsymbol{\nabla}}^{\boldsymbol{2}}\left(\frac{1}{|\vec{\boldsymbol{r}} - \vec{\boldsymbol{r}}_{\boldsymbol{0}}|}\right) = 0\,. \tag{5}$$

However, eq. (5) cannot be strictly true. After all, in section 1, we saw that a point charge produces an electric potential

$$\Phi(\vec{\boldsymbol{r}}) = \frac{q}{|\vec{\boldsymbol{r}} - \vec{\boldsymbol{r}}_{\boldsymbol{0}}|}\,,$$

and the Poisson equation implies that $\vec{\boldsymbol{\nabla}}^{\boldsymbol{2}}\Phi = 4\pi\rho \neq 0$. Indeed, using the results of section 1, given a point charge located at $\vec{\boldsymbol{r}}_{\boldsymbol{0}}$,

$$\vec{\boldsymbol{\nabla}}^{\boldsymbol{2}}\Phi(\vec{\boldsymbol{r}}) = q\vec{\boldsymbol{\nabla}}^{\boldsymbol{2}}\left(\frac{1}{|\vec{\boldsymbol{r}} - \vec{\boldsymbol{r}}_{\boldsymbol{0}}|}\right) = -4\pi\rho(\vec{\boldsymbol{r}}) = -4\pi q\delta^3(\vec{\boldsymbol{r}} - \vec{\boldsymbol{r}}_{\boldsymbol{0}})\,,$$

which yields

$$\vec{\boldsymbol{\nabla}}^{\boldsymbol{2}}\left(\frac{1}{|\vec{\boldsymbol{r}} - \vec{\boldsymbol{r}}_{\boldsymbol{0}}|}\right) = -4\pi\delta^3(\vec{\boldsymbol{r}} - \vec{\boldsymbol{r}}_{\boldsymbol{0}})\,. \tag{6}$$

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[1] It is standard practice to write $\vec{\boldsymbol{\nabla}}^{\boldsymbol{2}} \equiv \vec{\boldsymbol{\nabla}}^{\boldsymbol{2}}_{\boldsymbol{r}}$. That is, if no subscript appears, one assumes that derivatives are to be computed with respect to $\vec{\boldsymbol{r}}$.

Comparing eqs. (5) and (6), we see that our previous derivation is correct for all values of $\vec{\boldsymbol{r}} \neq \vec{\boldsymbol{r}}_{\mathbf{0}}$. However for $\vec{\boldsymbol{r}} = \vec{\boldsymbol{r}}_{\mathbf{0}}$, the inverse distance is singular, and hence the explicit computation of the Laplacian given above eq. (5) is suspect.

We can confirm the mathematical correctness of eq. (6) as follows. Again, it is convenient to work with the variable $\vec{\boldsymbol{R}}$, in which case, we have

$$\vec{\boldsymbol{\nabla}}^{\mathbf{2}}\left(\frac{1}{R}\right) = -4\pi\delta^3(\vec{\boldsymbol{R}})\,, \tag{7}$$

where $R \equiv |\vec{\boldsymbol{R}}|$. Let us integrate $\vec{\boldsymbol{\nabla}}^{\mathbf{2}}(1/R)$ over any volume V that contains the origin. We can divide up this volume into two pieces $V = V_a + V_b$, where V_a is a solid sphere of radius a whose center is the origin and V_b is the remaining part of the volume Then,

$$\int_V \vec{\boldsymbol{\nabla}}^{\mathbf{2}}\left(\frac{1}{R}\right) d^3R = \int_{V_a} \vec{\boldsymbol{\nabla}}^{\mathbf{2}}\left(\frac{1}{R}\right) d^3R + \int_{V_b} \vec{\boldsymbol{\nabla}}^{\mathbf{2}}\left(\frac{1}{R}\right) d^3R = \int_{V_a} \vec{\boldsymbol{\nabla}}^{\mathbf{2}}\left(\frac{1}{R}\right) d^3R\,,$$

since $\vec{\boldsymbol{\nabla}}^{\mathbf{2}}(1/R) = 0$ at all points in V_b since the latter excludes the origin. Using the divergence theorem of vector calculus,

$$\int_{V_a} \vec{\boldsymbol{\nabla}}^{\mathbf{2}}\left(\frac{1}{R}\right) d^3R = \int_{V_a} \vec{\boldsymbol{\nabla}}\cdot\vec{\boldsymbol{\nabla}}\left(\frac{1}{R}\right) d^3R = \oint_{S_a} \vec{\boldsymbol{\nabla}}\left(\frac{1}{R}\right)\cdot\hat{\boldsymbol{R}}\,ds\,,$$

where S_a is the closed spherical surface of radius a which constitutes the boundary of V_a. In particular, the outward normal to S_a is the unit radial vector $\hat{\boldsymbol{R}}$. The infinitesimal surface element is $ds = a^2 d\Omega$, where $d\Omega = \sin\theta d\theta d\phi$ is the usual differential solid angle element. Using

$$\vec{\boldsymbol{\nabla}}\left(\frac{1}{R}\right)\bigg|_{R=a} = \hat{\boldsymbol{R}}\frac{\partial}{\partial R}\left(\frac{1}{R}\right)\bigg|_{R=a} = -\frac{1}{a^2}\hat{\boldsymbol{R}}\,,$$

it follows that

$$\int_V \vec{\boldsymbol{\nabla}}^{\mathbf{2}}\left(\frac{1}{R}\right) d^3R = -\oint_{S_A} \hat{\boldsymbol{R}}\cdot\hat{\boldsymbol{R}}\frac{1}{a^2}\,a^2 d\Omega = -\oint_{S_A} d\Omega = -4\pi\,.$$

That is, we have shown that

$$\vec{\boldsymbol{\nabla}}^{\mathbf{2}}\left(\frac{1}{R}\right) = 0 \text{ for } R \neq 0 \qquad \text{and} \qquad \int_V \vec{\boldsymbol{\nabla}}^{\mathbf{2}}\left(\frac{1}{R}\right) d^3R = -4\pi\,,$$

for any volume V that contains the origin. The only "function" that satisfies these relations is

$$\vec{\boldsymbol{\nabla}}^{\mathbf{2}}\left(\frac{1}{R}\right) = -4\pi\delta^3(\vec{\boldsymbol{R}})\,,$$

since $\delta^3(\vec{\boldsymbol{R}}) = 0$ for any $\vec{\boldsymbol{R}} \neq 0$ and

$$\int_V \delta^3(\vec{\boldsymbol{R}})\,d^3R = 1\,,$$

for any volume V that contains the origin. Thus, we have confirmed the validity of eq. (7). More generally, we have established the result,

$$\boxed{\vec{\boldsymbol{\nabla}}^{\mathbf{2}}\left(\frac{1}{|\vec{\boldsymbol{r}} - \vec{\boldsymbol{r}}_{\mathbf{0}}|}\right) = -4\pi\delta^3(\vec{\boldsymbol{r}} - \vec{\boldsymbol{r}}_{\mathbf{0}})} \tag{8}$$

We finish this section by recording an important property of the delta function [which generalizes eq. (11.6) on p. 452 of Boas],

$$\int_V f(\vec{\boldsymbol{r}}')\,\delta^3(\vec{\boldsymbol{r}}-\vec{\boldsymbol{r}}')\,d^3r' = f(\vec{\boldsymbol{r}})\,, \qquad \text{where the point } \vec{\boldsymbol{r}} \text{ lies within the volume } V\,. \tag{9}$$

This is easy to understand since the delta function vanishes everywhere except at the point where $\vec{\boldsymbol{r}}' = \vec{\boldsymbol{r}}$. Of course, if $f(\vec{\boldsymbol{r}}) = 1$ for all $\vec{\boldsymbol{r}}$, then eq. (9) yields the well known result

$$\int_V \delta^3(\vec{\boldsymbol{r}}-\vec{\boldsymbol{r}}')\,d^3r' = 1\,, \qquad \text{where the point } \vec{\boldsymbol{r}} \text{ lies within the volume } V\,.$$

3. Solutions to the Poisson Equation

We wish to solve the Poisson equation, eq. (3), given a known charge distribution $\rho(\vec{\boldsymbol{r}})$ that is nonzero over some finite volume of space, subject to boundary conditions (typically taken to be Dirichlet, in which Φ is specified over some closed surface or Neumann where $\vec{\boldsymbol{E}} = -\vec{\boldsymbol{\nabla}}\Phi$ is specified over some closed surface). The solution will take the form,

$$\Phi(\vec{\boldsymbol{r}}) = \Phi_p(\vec{\boldsymbol{r}}) + \Phi_c(\vec{\boldsymbol{r}})\,, \tag{10}$$

where $\Phi_p(\vec{\boldsymbol{r}})$ is a particular solution to the Poisson equation and $\Phi_c(\vec{\boldsymbol{r}})$ is the (complementary) solution to the Laplace equation, $\vec{\boldsymbol{\nabla}}^2\Phi_c(\vec{\boldsymbol{r}}) = 0$. In defining the particular solution, we shall impose the condition that

$$\lim_{r\to\infty}\Phi_p(\vec{\boldsymbol{r}}) = 0\,, \tag{11}$$

which can be viewed as a boundary condition that states that $\Phi_p(\vec{\boldsymbol{r}})$ vanishes on the surface of a sphere of radius r in the limit of $r \to \infty$. Then

$$\Phi_p(\vec{\boldsymbol{r}}) = \int \frac{\rho(\vec{\boldsymbol{r}}')}{|\vec{\boldsymbol{r}}-\vec{\boldsymbol{r}}'|}\,d^3r'\,, \tag{12}$$

where the integration is taken over all of three-dimensional space. To prove that $\Phi_p(\vec{\boldsymbol{r}})$ satisfies the Poisson equation subject to eq. (11), we first note that as $r \to \infty$, we have $|\vec{\boldsymbol{r}}-\vec{\boldsymbol{r}}'| = r[1+\mathcal{O}(1/r)]$ so that

$$\lim_{r\to\infty}\Phi_p(\vec{\boldsymbol{r}}) = \lim_{r\to\infty}\int \frac{\rho(\vec{\boldsymbol{r}}')}{|\vec{\boldsymbol{r}}-\vec{\boldsymbol{r}}'|}\,d^3r' = \lim_{r\to\infty}\frac{1}{r}\int \rho(\vec{\boldsymbol{r}}')d^3r' + \mathcal{O}\left(\frac{1}{r^2}\right) = \lim_{r\to\infty}\frac{q}{r} + \mathcal{O}\left(\frac{1}{r^2}\right) = 0\,, \tag{13}$$

where we have used eq. (4), under the assumption that the charge distribution is restricted to a finite region of space. Next, we compute the Laplacian of $\Phi_p(\vec{\boldsymbol{r}})$,

$$\begin{aligned}\vec{\boldsymbol{\nabla}}^2\Phi_p(\vec{\boldsymbol{r}}) &= \vec{\boldsymbol{\nabla}}^2\int \frac{\rho(\vec{\boldsymbol{r}}')}{|\vec{\boldsymbol{r}}-\vec{\boldsymbol{r}}'|}\,d^3r' = \int \rho(\vec{\boldsymbol{r}}')\vec{\boldsymbol{\nabla}}^2\left(\frac{1}{|\vec{\boldsymbol{r}}-\vec{\boldsymbol{r}}'|}\right)d^3r' \\ &= -4\pi\int \rho(\vec{\boldsymbol{r}}')\delta^3(\vec{\boldsymbol{r}}-\vec{\boldsymbol{r}}')d^3r' = -4\pi\rho(\vec{\boldsymbol{r}})\,, \end{aligned} \tag{14}$$

where we have used eq. (8). Note that $\vec{\nabla}^2$ involves derivatives with respect to $\vec{r}$, so that in applying the Laplacian, the variable $\vec{r}\,'$ (which is a dummy integration variable) is treated as being fixed. Thus, we have verified that $\Phi_p(\vec{r})$ is a solution to the Poisson equation.

Indeed, $\Phi_p(\vec{r})$ is the unique solution to the Poisson equation, which is valid at all points in space, subject to eq. (11). More general boundary value problems would involve solving the Poisson equation in a restricted region of space, V. In this case, we must specify the boundary conditions on the closed surface S of V. The solution is then given by:

$$\Phi(\vec{r}) = \Phi_c(\vec{r}) + \int_V \frac{\rho(\vec{r}\,')}{|\vec{r}-\vec{r}\,'|}\, d^3r' \,, \tag{15}$$

where $\Phi_c(\vec{r})$ is a solution to the Laplace equation, which is chosen such that the boundary conditions are satisfied when applied to the *complete* solution to the problem, $\Phi(\vec{r})$.

4. The inverse Laplacian and the Green function

Consider the solution to the Poisson equation, which is valid at all points in space, subject to eq. (11),

$$\vec{\nabla}^2\Phi(\vec{r}) = -4\pi\rho(\vec{r})\,, \tag{16}$$

where $\rho(\vec{r})$ is nonzero only over some finite region in space. In fact, this last assumption is stronger than is necessary. It is sufficient to assume that $\rho(\vec{r}) \to 0$ as $r \to \infty$ fast enough such that the volume integral of $\rho(\vec{r})$ over all space converges. Then, as discussed in Section 3, the solution to the Poisson equation is unique. That is, the solution to the Poisson equation is given by eq. (15) with $\Phi_c(\vec{r}) = 0$. Equivalently, $\Phi(\vec{r}) = \Phi_p(\vec{r})$, where $\Phi_p(\vec{r})$ is given by eq. (12).

Under the stated conditions above, it is tempting to derive the solution to the Poisson equation by introducing the inverse Laplacian, $\vec{\nabla}^{-2}$. Operating with the inverse Laplacian on eq. (16) yields,

$$\vec{\nabla}^{-2}\vec{\nabla}^2\Phi(\vec{r}) = -4\pi\vec{\nabla}^{-2}\rho(\vec{r})\,.$$

Clearly, one should define $\vec{\nabla}^{-2}\vec{\nabla}^2$ to be the identity operator, in which case we would conclude that

$$\Phi(\vec{r}) = -4\pi\vec{\nabla}^{-2}\rho(\vec{r})\,. \tag{17}$$

Comparing this with $\Phi(\vec{r}) = \Phi_p(\vec{r})$, where $\Phi_p(\vec{r})$ is given by eq. (12), it follows that we should identify

$$\boxed{\vec{\nabla}^{-2}\rho(\vec{r}) = -\frac{1}{4\pi}\int \frac{\rho(\vec{r}\,')}{|\vec{r}-\vec{r}\,'|}\, d^3r'} \tag{18}$$

Plugging eq. (18) back into eq. (17) yields

$$\Phi(\vec{r}) = \int \frac{\rho(\vec{r}\,')}{|\vec{r}-\vec{r}\,'|}\, d^3r' \,, \tag{19}$$

as expected.

The definition of the inverse Laplacian given in eq. (18) shows that this operator acts nonlocally. That is, the value of $\vec{\nabla}^{-2}\rho(\vec{r})$ at the point $\vec{r}$ depends on $\rho(\vec{r}\,')$ evaluated at all points in space. This should not be surprising to you. After all, the antiderivative of calculus is an integral! More importantly, the definition of the inverse Laplacian requires an assumption about the space of functions on which it acts. In the present case, we have required that the space of functions should only include twice differentiable functions that vanish sufficiently fast at infinity. To check that the definition of the inverse Laplacian given in eq. (18) is sensible, we perform the following two computations:

$$\begin{aligned}\vec{\nabla}^2\vec{\nabla}^{-2}\rho(\vec{r}) &= -\frac{1}{4\pi}\vec{\nabla}^2\int\frac{\rho(\vec{r}\,')}{|\vec{r}-\vec{r}\,'|}\,d^3r' = -\frac{1}{4\pi}\int\rho(\vec{r}\,')\vec{\nabla}^2\left(\frac{1}{|\vec{r}-\vec{r}\,'|}\right)d^3r' \\ &= \int\rho(\vec{r}\,')\delta^3(\vec{r}-\vec{r}\,')d^3r' = \rho(\vec{r})\,,\end{aligned}$$

after using eq. (9), and

$$\begin{aligned}\vec{\nabla}^{-2}\left[\vec{\nabla}^2\rho(\vec{r})\right] &= -\frac{1}{4\pi}\int\frac{\vec{\nabla}'^2\rho(\vec{r}\,')}{|\vec{r}-\vec{r}\,'|}\,d^3r' = -\frac{1}{4\pi}\int\rho(\vec{r}\,')\vec{\nabla}'^2\left(\frac{1}{|\vec{r}-\vec{r}\,'|}\right)d^3r' \\ &= \int\rho(\vec{r}\,')\delta^3(\vec{r}-\vec{r}\,')d^3r' = \rho(\vec{r})\,,\end{aligned} \tag{20}$$

where $\vec{\nabla}'^2$ is the Laplacian that involves derivatives with respect to $\vec{r}\,'$. Note that in deriving eq. (20) we integrated by parts twice using Green's second identity (details are provided in the Appendix). In particular, we took $\psi=\rho$ and $\phi=1/|\vec{r}-\vec{r}\,'|$ in eq. (39). Indeed, as both $\rho(\vec{r}\,')$ and $1/|\vec{r}-\vec{r}\,'|$ vanish at the surface of infinity, we are justified in setting the right hand side of eq. (38) to zero. Thus, we have shown that eq. (18), subject to restrictions on $\rho(\vec{r})$ at infinity, satisfies

$$\vec{\nabla}^2\vec{\nabla}^{-2}\rho(\vec{r}) = \vec{\nabla}^{-2}\vec{\nabla}^2\rho(\vec{r}) = \rho(\vec{r})\,,$$

which confirms that both $\vec{\nabla}^2\vec{\nabla}^{-2}$ and $\vec{\nabla}^2\vec{\nabla}^{-2}$ are equivalent to the identity operator.

The inverse Laplacian can also be used to determine the Green function of the Poisson equation. First we assume that the potential vanishes sufficiently fast at infinity, as discussed below eq. (11). We define the Green function $G(\vec{r},\vec{r}\,')$ to be the solution of

$$\vec{\nabla}^2 G(\vec{r},\vec{r}\,') = -4\pi\delta^3(\vec{r}-\vec{r}\,')\,. \tag{21}$$

The factor of -4π is conventional (although not the convention adopted by Boas). Then,

$$G(\vec{r},\vec{r}\,') = -4\pi\vec{\nabla}^{-2}\delta^3(\vec{r}-\vec{r}\,') = \int\frac{\delta^3(\vec{r}\,''-\vec{r}\,')}{|\vec{r}-\vec{r}\,''|}d^3r'' = \frac{1}{|\vec{r}-\vec{r}\,'|}\,. \tag{22}$$

Thus, the inverse Laplacian provides a very quick derivation of the Green function. The interpretation of the Green function is clear—it is the potential that arises due to the presence of a point charge located at $\vec{r}\,'$. The utility of the Green function is that it can be used to construct the potential for an arbitrary charge density via

$$\Phi(\vec{r}) = \int G(\vec{r},\vec{r}\,')\rho(\vec{r}\,')d^3r'\,, \tag{23}$$

since eq. (23) implies that $\Phi(\vec{\boldsymbol{r}})$ satisfies the Poisson equation, i.e.,

$$\vec{\boldsymbol{\nabla}}^{\mathbf{2}}\Phi(\vec{\boldsymbol{r}}) = \int \rho(\vec{\boldsymbol{r}}')\vec{\boldsymbol{\nabla}}^{\mathbf{2}}G(\vec{\boldsymbol{r}},\vec{\boldsymbol{r}}')\,d^3r' = -4\pi\int \rho(\vec{\boldsymbol{r}})\delta^3(\vec{\boldsymbol{r}}-\vec{\boldsymbol{r}}')\,d^3r' = -4\pi\rho(\vec{\boldsymbol{r}})\,.$$

Another interpretation of the Green function can be ascertained from eq. (22). The Dirac delta function is the function space analog of the Kronecker delta δ_{ij}. Thus, the Dirac delta function is an infinite dimensional matrix corresponding to the identity matrix, where $\delta^3(\vec{\boldsymbol{r}}-\vec{\boldsymbol{r}}')$ are the matrix elements of this infinite dimensional matrix. Apart from the overall factor of -4π (which is a matter of convention), $G(\vec{\boldsymbol{r}},\vec{\boldsymbol{r}}')$ are the matrix elements of the infinite dimensional matrix that represents the inverse Laplacian.

In more general boundary value problems, one must solve the Poisson equation in a restricted region of space, V. In this case, we must specify the boundary conditions on the closed surface S of V. The corresponding Green function is still a solution to eq. (21), but it now must also satisfy the relevant boundary conditions. Thus, in analogy to eq. (15), the Green function takes the form

$$G(\vec{\boldsymbol{r}},\vec{\boldsymbol{r}}') = F(\vec{\boldsymbol{r}},\vec{\boldsymbol{r}}') + \frac{1}{|\vec{\boldsymbol{r}}-\vec{\boldsymbol{r}}'|}\,, \qquad (24)$$

where $F(\vec{\boldsymbol{r}},\vec{\boldsymbol{r}}')$ is a solution to the Laplace equation that is adjusted in order that $G(\vec{\boldsymbol{r}},\vec{\boldsymbol{r}}')$ satisfy the relevant boundary conditions. In this case, eq. (23) yields

$$\Phi(\vec{\boldsymbol{r}}) = \int_V G(\vec{\boldsymbol{r}},\vec{\boldsymbol{r}}')\rho(\vec{\boldsymbol{r}}')d^3r' = \int_V F(\vec{\boldsymbol{r}},\vec{\boldsymbol{r}}')\rho(\vec{\boldsymbol{r}}')d^3r' + \int_V \frac{\rho(\vec{\boldsymbol{r}}')}{|\vec{\boldsymbol{r}}-\vec{\boldsymbol{r}}'|}d^3r'\,.$$

Comparing with eq. (15), we identify

$$\Phi_c(\vec{\boldsymbol{r}}) = \int_V F(\vec{\boldsymbol{r}},\vec{\boldsymbol{r}}')\rho(\vec{\boldsymbol{r}}')d^3r'\,. \qquad (25)$$

A concrete example is provided by the Green function for the Laplace equation, denoted by $G_D(\vec{\boldsymbol{r}},\vec{\boldsymbol{r}}')$, that satisfies Dirichlet boundary conditions on the surface S that caps the volume V. That is, we wish to choose $F(\vec{\boldsymbol{r}},\vec{\boldsymbol{r}}')$ in eq. (24) such that

$$G_D(\vec{\boldsymbol{r}},\vec{\boldsymbol{r}}') = 0\,, \qquad \text{for } \vec{\boldsymbol{r}}' \text{ on } S\,. \qquad (26)$$

To proceed, we make use of Green's second identity, which is presented in Appendix A. For convenience, we rewrite this identity below,[2]

$$\int_V \bigl[\phi(\vec{\boldsymbol{r}}')\vec{\boldsymbol{\nabla}}'^{\mathbf{2}}\psi(\vec{\boldsymbol{r}}') - \psi(\vec{\boldsymbol{r}}')\vec{\boldsymbol{\nabla}}'^{\mathbf{2}}\phi(\vec{\boldsymbol{r}}')\bigr]d^3r' = \oint_S \left(\phi(\vec{\boldsymbol{r}}')\frac{\partial\psi}{\partial n'} - \psi(\vec{\boldsymbol{r}}')\frac{\partial\phi}{\partial n'}\right)da'\,, \qquad (27)$$

where we have used primed letters for the integration variables. Choose $\phi = \Phi(\vec{\boldsymbol{r}}')$ and $\psi = G_D(\vec{\boldsymbol{r}},\vec{\boldsymbol{r}}')$ in eq. (27) above, where Φ satisfies the Poisson equation [cf. eq. (3)]. Then, using

$$\vec{\boldsymbol{\nabla}}'^{\mathbf{2}}G_D(\vec{\boldsymbol{r}},\vec{\boldsymbol{r}}') = -4\pi\delta^3(\vec{\boldsymbol{r}}-\vec{\boldsymbol{r}}')\,,$$

[2]The normal derivative of $\phi(\vec{\boldsymbol{r}}')$ defined on a surface S is $\partial\psi/\partial n' \equiv \hat{\boldsymbol{n}}'\boldsymbol{\cdot}\vec{\boldsymbol{\nabla}}'\psi$.

which follows from eqs. (21) and (36), we see that

$$\int_V \Phi(\boldsymbol{\vec{r}'})\boldsymbol{\vec{\nabla}'^2} G_D(\boldsymbol{\vec{r}},\boldsymbol{\vec{r}'})\,d^3r' = -4\pi\int_V \Phi(\boldsymbol{\vec{r}'})\delta^3(\boldsymbol{\vec{r}}-\boldsymbol{\vec{r}'})\,d^3r' = -4\pi\Phi(\boldsymbol{\vec{r}})\,,$$

where we have used the well-known properties of the delta function to perform the integration above. Moreover, since $\boldsymbol{\vec{\nabla}'^2}\Phi(\boldsymbol{\vec{r}'}) = -4\pi\rho(\boldsymbol{\vec{r}'})$, the left hand side of eq. (27) reduces to

$$-4\pi\left\{\Phi(\boldsymbol{\vec{r}}) - \int_V G_D(\boldsymbol{\vec{r}},\boldsymbol{\vec{r}'})\rho(\boldsymbol{\vec{r}'})\,d^3r'\right\}\,.$$

Thus, using the boundary condition specified in eq. (26), we see that eq. (27) with $\phi = \Phi(\boldsymbol{\vec{r}'})$ and $\psi = G_D(\boldsymbol{\vec{r}},\boldsymbol{\vec{r}'})$ reduces to

$$\Phi(\boldsymbol{\vec{r}}) = \int_V G_D(\boldsymbol{\vec{r}},\boldsymbol{\vec{r}'})\rho(\boldsymbol{\vec{r}'})\,d^3r' - \frac{1}{4\pi}\oint_S \Phi(\boldsymbol{\vec{r}'})\frac{\partial G_D(\boldsymbol{\vec{r}},\boldsymbol{\vec{r}'})}{\partial n'}\,da'\,. \tag{28}$$

We identify the second term on the right hand side of eq. (28) as $\Phi_c(\boldsymbol{\vec{r}})$, which can then be used in eq. (25) to determine $F(\boldsymbol{\vec{r}},\boldsymbol{\vec{r}'})$.

The inverse Laplacian was defined in eq. (18) under the assumption that it acts on functions (defined at all points in space) that vanish sufficiently fast at infinity. In contrast, if the functions are defined only in a restricted region of space V, then the inverse Laplacian is ill-defined unless one imposes boundary conditions on the closed surface S of V. This can be understood as follows. If we solve the Laplace equation inside V, we find non-trivial solutions, denoted by $\Phi_c(\boldsymbol{\vec{r}})$ in eq. (10). That is, the Laplacian possesses an eigenfunction $\Phi_c(\boldsymbol{\vec{r}})$ with corresponding eigenvalue equal to zero. This immediately implies that $\boldsymbol{\vec{\nabla}^{-2}}$ is ill-defined; otherwise one would obtain eq. (18) instead of the correct result given in eq. (15).[3] This means that eq. (17) does not determine $\Phi(\boldsymbol{\vec{r}})$ uniquely. This is not surprising, as we have not yet specified the boundary conditions on S. However, once we specify these conditions, $\Phi(\boldsymbol{\vec{r}})$ is uniquely determined. This means that the definition of $\boldsymbol{\vec{\nabla}^{-2}}$ [which generalizes eq. (18)] becomes well-defined. This is not surprising, since we know that the form of the Green function depends in detail on the boundary conditions that are applied, which determines $F(\boldsymbol{\vec{r}},\boldsymbol{\vec{r}'})$ as indicated in eq. (24).

5. Derivation of the Green function by Fourier transforms

The derivation of the Green function in eq. (22) is very slick. In this section, I will provide another technique for computing the Green function of the Poisson equation that employs the Fourier transform. We need to generalize eq. (12.2) on p. 379, which exhibits the Fourier transform in one dimension. In three dimensions, we define the Fourier transform of the function $f(\boldsymbol{\vec{r}})$ by

$$g(\boldsymbol{\vec{k}}) = \int f(\boldsymbol{\vec{r}})e^{i\boldsymbol{\vec{k}}\cdot\boldsymbol{\vec{r}}}\,d^3r\,. \tag{29}$$

[3]Consider the analogous case of a finite dimensional operator and its matrix representation M. If M has a zero eigenvalue, then its determinant vanishes (since $\det M$ is the product of its eigenvalues), in which case M^{-1} is ill-defined.

If we know $g(\vec{\boldsymbol{k}})$, then we can compute $f(\vec{\boldsymbol{r}})$ using

$$f(\vec{\boldsymbol{r}}) = \frac{1}{(2\pi)^3}\int g(\vec{\boldsymbol{k}})e^{-i\vec{\boldsymbol{k}}\cdot\vec{\boldsymbol{r}}}\,d^3k\,. \tag{30}$$

We shall apply these results to the defining equation of the Green function [cf. eq. (21)]:

$$\vec{\boldsymbol{\nabla}}^{\boldsymbol{2}}G(\vec{\boldsymbol{r}},\vec{\boldsymbol{r}}') = -4\pi\delta^3(\vec{\boldsymbol{r}}-\vec{\boldsymbol{r}}')\,. \tag{31}$$

We now take the Fourier transform of both sides of this equation,

$$\int[\vec{\boldsymbol{\nabla}}^{\boldsymbol{2}}G(\vec{\boldsymbol{r}},\vec{\boldsymbol{r}}')]e^{i\vec{\boldsymbol{k}}\cdot\vec{\boldsymbol{r}}}\,d^3r = -4\pi\int\delta^3(\vec{\boldsymbol{r}}-\vec{\boldsymbol{r}}')\,e^{i\vec{\boldsymbol{k}}\cdot\vec{\boldsymbol{r}}}\,d^3r\,. \tag{32}$$

Using eq. (9), we immediately obtain,

$$\int\delta^3(\vec{\boldsymbol{r}}-\vec{\boldsymbol{r}}')\,e^{i\vec{\boldsymbol{k}}\cdot\vec{\boldsymbol{r}}}\,d^3r = e^{i\vec{\boldsymbol{k}}\cdot\vec{\boldsymbol{r}}'}\,.$$

To evaluate the left hand side of eq. (9), we integrate by parts twice using Green's second identity (for details, see the Appendix). When eq. (38) is applied to eq. (32), we identify $\psi = G(\vec{\boldsymbol{r}},\vec{\boldsymbol{r}}')$ and $\phi = e^{i\vec{\boldsymbol{k}}\cdot\vec{\boldsymbol{r}}}$. Since $G(\vec{\boldsymbol{r}},\vec{\boldsymbol{r}}')$ and $\vec{\boldsymbol{\nabla}}G(\vec{\boldsymbol{r}},\vec{\boldsymbol{r}}')$ vanish at infinity, we are justified in setting the right hand side of eq. (38) to zero. Hence, eq. (39) yields

$$\int[\vec{\boldsymbol{\nabla}}^{\boldsymbol{2}}G(\vec{\boldsymbol{r}},\vec{\boldsymbol{r}}')]e^{i\vec{\boldsymbol{k}}\cdot\vec{\boldsymbol{r}}}\,d^3r = \int G(\vec{\boldsymbol{r}},\vec{\boldsymbol{r}}')[\vec{\boldsymbol{\nabla}}^{\boldsymbol{2}}e^{i\vec{\boldsymbol{k}}\cdot\vec{\boldsymbol{r}}}]\,d^3r\,.$$

Using

$$\vec{\boldsymbol{\nabla}}^{\boldsymbol{2}}e^{i\vec{\boldsymbol{k}}\cdot\vec{\boldsymbol{r}}} = -k^2e^{i\vec{\boldsymbol{k}}\cdot\vec{\boldsymbol{r}}}\,,$$

we conclude that

$$\int[\vec{\boldsymbol{\nabla}}^{\boldsymbol{2}}G(\vec{\boldsymbol{r}},\vec{\boldsymbol{r}}')]e^{i\vec{\boldsymbol{k}}\cdot\vec{\boldsymbol{r}}}\,d^3r = -k^2\int G(\vec{\boldsymbol{r}},\vec{\boldsymbol{r}}')e^{i\vec{\boldsymbol{k}}\cdot\vec{\boldsymbol{r}}}\,d^3r\,.$$

Hence, eq. (32) yields

$$\int G(\vec{\boldsymbol{r}},\vec{\boldsymbol{r}}')e^{i\vec{\boldsymbol{k}}\cdot\vec{\boldsymbol{r}}}\,d^3r = \frac{4\pi}{k^2}e^{i\vec{\boldsymbol{k}}\cdot\vec{\boldsymbol{r}}'}\,. \tag{33}$$

We have succeeded in evaluating the Fourier transform of the Green function, which we shall denote by

$$g(\vec{\boldsymbol{k}}) \equiv \int G(\vec{\boldsymbol{r}},\vec{\boldsymbol{r}}')e^{i\vec{\boldsymbol{k}}\cdot\vec{\boldsymbol{r}}}\,d^3r\,.$$

Indeed, you can now see the utility of employing the Fourier transform. By taking the Fourier transform of the partial differential equation given in eq. (31), we have converted it into an algebraic equation,

$$-k^2g(\vec{\boldsymbol{k}}) = -4\pi e^{i\vec{\boldsymbol{k}}\cdot\vec{\boldsymbol{r}}'}\,.$$

The solution to this algebraic equation is trivial, namely

$$g(\vec{\boldsymbol{k}}) = \frac{4\pi}{k^2}e^{i\vec{\boldsymbol{k}}\cdot\vec{\boldsymbol{r}}'}\,, \tag{34}$$

which we recognize as eq. (33) above.

Thus, using eqs. (29) and (30), we can determine the Green function itself. In eq. (33), $G(\vec{\boldsymbol{r}}, \vec{\boldsymbol{r}}')$ plays the role of $f(\vec{\boldsymbol{r}})$ in eq. (29) and $g(\vec{\boldsymbol{k}})$ is given by eq. (34).[4] We can therefore use eq. (30) to obtain

$$G(\vec{\boldsymbol{r}}, \vec{\boldsymbol{r}}') = \frac{1}{(2\pi)^3} \int g(\vec{\boldsymbol{k}}) e^{-i\vec{\boldsymbol{k}}\cdot\vec{\boldsymbol{r}}}\, d^3k = \frac{4\pi}{(2\pi)^3} \int \frac{e^{-i\vec{\boldsymbol{k}}\cdot(\vec{\boldsymbol{r}}-\vec{\boldsymbol{r}}')}}{k^2}\, d^3k\,. \tag{35}$$

Observe that $G(\vec{\boldsymbol{r}}, \vec{\boldsymbol{r}}')$ is a function of $\vec{\boldsymbol{r}} - \vec{\boldsymbol{r}}'$. This is perhaps not too surprising in light of the definition of the Green function given in eq. (31), and it can be attributed to translational invariance.[5]

Thus, we can write

$$G(\vec{\boldsymbol{r}}, \vec{\boldsymbol{r}}') = G(\vec{\boldsymbol{r}} - \vec{\boldsymbol{r}}', 0)\,. \tag{36}$$

In particular, we can compute $G(\vec{\boldsymbol{r}}, \vec{\boldsymbol{r}}')$ in eq. (35) by setting $\vec{\boldsymbol{r}}' = 0$. When we have finished, we can restore $\vec{\boldsymbol{r}}'$ using eq. (36).

If we denote $G(\vec{\boldsymbol{r}}) \equiv G(\vec{\boldsymbol{r}}, 0)$ then eq. (35) yields

$$G(\vec{\boldsymbol{r}}) = \frac{1}{2\pi^2} \int \frac{e^{-i\vec{\boldsymbol{k}}\cdot\vec{\boldsymbol{r}}}}{k^2}\, d^3k\,.$$

We can evaluate this integral using spherical coordinates. Without loss of generality, we can set up a coordinate system in which $\vec{\boldsymbol{r}}$ lies along the z-axis and $\vec{\boldsymbol{k}}$ points in some direction with polar angle θ and azimuthal angle ϕ with respect to the direction of $\vec{\boldsymbol{r}}$. We write $d^3k = k^2\, dk\, d\cos\theta\, d\phi$ and $\vec{\boldsymbol{k}}\cdot\vec{\boldsymbol{r}} = kr\cos\theta$. Hence, assuming that $r \neq 0$,[6]

$$\begin{aligned}
G(\vec{\boldsymbol{r}}) &= \frac{1}{2\pi^2} \int_0^\infty k^2\, dk \int_{-1}^{1} d\cos\theta \int_0^{2\pi} d\phi\, \frac{e^{-ikr\cos\theta}}{k^2} \\
&= \frac{1}{2\pi^2} \cdot (2\pi) \int_0^\infty dk \int_{-1}^{1} e^{-ikr\cos\theta}\, d\cos\theta \\
&= \frac{1}{\pi} \int_0^\infty dk \frac{e^{-ikr\cos\theta}}{-ikr}\bigg|_{-1}^{1} = \frac{1}{\pi r} \int_0^\infty \frac{dk}{k} \left(\frac{e^{-ikr} - e^{ikr}}{-i} \right) \\
&= \frac{2}{\pi r} \int_0^\infty \frac{\sin kr}{k}\, dk\,,
\end{aligned} \tag{37}$$

after recognizing that $\sin kr = (e^{ikr} - e^{-ikr})/(2i)$.

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[4]Note that in this analysis, $\vec{\boldsymbol{r}}'$ simply goes along for the ride.

[5]Translational invariance in this context implies that we can translate (i.e. move) all position vectors in the world by a constant vector $\vec{\boldsymbol{a}}$, i.e. $\vec{\boldsymbol{r}} \to \vec{\boldsymbol{r}} + \vec{\boldsymbol{a}}$, without affecting our equations.

[6]If $r = 0$ then we obtain

$$G(0) = \frac{1}{\pi} \int_0^\infty dk \int_{-1}^{1} d\cos\theta = \frac{2}{\pi} \int_0^\infty dk\,,$$

which diverges. Thus the Green function is not defined at this point.

Using the integral derived on pp. 690–691 of Boas,

$$\int_{-\infty}^{\infty} \frac{\sin x}{x}\, dx = \pi\,,$$

it follows that

$$\int_{0}^{\infty} \frac{\sin x}{x}\, dx = \tfrac{1}{2}\pi\,,$$

since $\sin x/x$ is an even function of x. Setting $x = kr$, where $r > 0$ (since r is a radial variable that we have assumed above to be non-zero), and noting that $dx/x = dk/k$, we conclude that

$$\int_{0}^{\infty} \frac{\sin kr}{k}\, dk = \tfrac{1}{2}\pi\,.$$

Inserting this result into eq. (37) and identifying $r = |\vec{\boldsymbol{r}}|$, we end up with

$$G(\vec{\boldsymbol{r}}) = \frac{1}{|\vec{\boldsymbol{r}}|}\,, \qquad \text{for } r \neq 0\,.$$

Finally, using eq. (36), we conclude that

$$G(\vec{\boldsymbol{r}}, \vec{\boldsymbol{r}}\,') = \frac{1}{|\vec{\boldsymbol{r}} - \vec{\boldsymbol{r}}\,'|}\,, \qquad \text{for } \vec{\boldsymbol{r}} \neq \vec{\boldsymbol{r}}\,'\,,$$

which confirms the result previously obtained in eq. (22) after a single line of calculation! Of course, this comparison is not really fair, since the origin of eq. (22) can be traced to eq. (12), which contains within it the Green function that one is claiming to derive. The benefit of the derivation by Fourier transforms given in this section is that the Green function has truly been obtained from scratch without prior knowledge of its form.

Appendix: Green's second identity

Green's second identity, introduced in problem 6.10–16 on p. 324 of Boas, is given by:

$$\int_V (\phi \vec{\boldsymbol{\nabla}}^{\boldsymbol{2}} \psi - \psi \vec{\boldsymbol{\nabla}}^{\boldsymbol{2}} \phi) d^3 r = \oint_S (\phi \vec{\boldsymbol{\nabla}} \psi - \psi \vec{\boldsymbol{\nabla}} \phi) \boldsymbol{\cdot} \hat{\boldsymbol{n}} da\,. \tag{38}$$

If V is the volume of all space, then S is the surface at infinity. In many applications, one can show that the integrand $\phi \vec{\boldsymbol{\nabla}} \psi - \psi \vec{\boldsymbol{\nabla}} \phi$ vanishes at the surface of infinity. In this case, the right hand side of eq. (38) vanishes, and it follows that

$$\int \phi \vec{\boldsymbol{\nabla}}^{\boldsymbol{2}} \psi \, d^3 r = \int \psi \vec{\boldsymbol{\nabla}}^{\boldsymbol{2}} \phi \, d^3 r\,. \tag{39}$$