Unit 2-3-S: Eigenfunction Expansion for the Green's Function

Suppose $\mathbb{D}$ is some linear differential operator, for example ∇^2. Solutions to the equation,

$$\mathbb{D}\psi(\mathbf{r}) = -4\pi f(\mathbf{r}) \tag{2.3.S.1}$$

can be found if one knows the Green's function for the operator, which is the solution to the problem with a point source,

$$\mathbb{D}G(\mathbf{r},\mathbf{r}') = -4\pi\delta(\mathbf{r}-\mathbf{r}') \qquad \text{here, } \mathbb{D} \text{ operates on the variable } \mathbf{r}\text{, and not on } \mathbf{r}' \tag{2.3.S.2}$$

Then the solution for the source $f(\mathbf{r})$ will be

$$\psi(\mathbf{r}) = \int d^3r'\, G(\mathbf{r},\mathbf{r}')f(\mathbf{r}') \tag{2.3.S.3}$$

If we need to solve for $\psi(\mathbf{r})$ subject to certain boundary conditions, then we can always add to the Green's function a $\phi(\mathbf{r})$ such that $\mathbb{D}\phi(\mathbf{r}) = 0$ in the desired region, and then choose $\phi(\mathbf{r})$ accordingly so that $G(\mathbf{r},\mathbf{r}')$ will satisfy the desired boundary conditions, as we did when constructing the Dirichlet and Neumann Green's functions for ∇^2.

One way to find $G(\mathbf{r},\mathbf{r}')$ is to find the eigenvalues and eigenfunctions of $\mathbb{D}$,

$$\mathbb{D}\psi_n(\mathbf{r}) = \lambda_n\psi_n(\mathbf{r}) \qquad \text{where } \psi_n(\mathbf{r}) \text{ is the eigenfunction and } \lambda_n \text{ is the eigenvalue} \tag{2.3.S.4}$$

Depending on the problem the spectrum of eigenvalues might be discrete or might be continuous.

[Note: when we solved Laplace's equation by separation of variables in spherical coordinates (and similarly in rectangular and cylindrical coordinates), what we wound up doing was solving the eigenvalue problem for the radial r, θ, and ϕ pieces of the differential operator ∇^2.]

In many cases (one would need to prove it for the particular operator $\mathbb{D}$) the eigenfunctions $\psi_n(\mathbf{r})$ form an orthogonal and complete set of basis functions over the region of interest (i.e. in the volume in which one is seeking a solution).

$$\underline{\text{orthogonal}} \quad \Rightarrow \quad \int_V d^3r\, \psi_m^*(\mathbf{r})\psi_n(\mathbf{r}) = \delta_{mn} \tag{2.3.S.5}$$

$$\underline{\text{complete}} \quad \Rightarrow \quad f(\mathbf{r}) = \sum_n a_n\psi_n(\mathbf{r}) \quad \text{for some coefficients } a_n \tag{2.3.S.6}$$

Then any function $f(\mathbf{r})$ can be expanded in a linear combination of the ψ_n, and the expansion coefficients a_n are determined by,

$$\int_V d^3r\, f(\mathbf{r})\psi_m^*(\mathbf{r}) = \sum_n a_n \int_V d^3r\, \psi_m^*(\mathbf{r})\psi_n(\mathbf{r}) = \sum_n a_n\delta_{mn} = a_m \tag{2.3.S.7}$$

So

$$\boxed{a_m = \int_V d^3r\, f(\mathbf{r})\psi^*(\mathbf{r})} \quad \text{gives the "Fourier" coefficient of } f(\mathbf{r}) \text{ in the basis } \phi_n(\mathbf{r}) \tag{2.3.S.8}$$

In particular, the function $\delta(\mathbf{r}-\mathbf{r}')$ can be expanded as,

$$\delta(\mathbf{r}-\mathbf{r}') = \sum_n a_n\psi_n(\mathbf{r}) \quad \text{where} \quad a_n = \int_V d^3r\, \delta(\mathbf{r}-\mathbf{r}')\psi_n^*(\mathbf{r}) = \psi_n^*(\mathbf{r}') \tag{2.3.S.9}$$

so,

$$\delta(\mathbf{r}-\mathbf{r}') = \sum_n \psi_n^*(\mathbf{r}')\psi_n(\mathbf{r}) \tag{2.3.S.10}$$

Now we can solve for the Green's function! Expand $G(\mathbf{r}, \mathbf{r}')$, as a function of $\mathbf{r}$, as a series in the $\psi_n(\mathbf{r})$,

$$G(\mathbf{r}, \mathbf{r}') = \sum_n a_n \psi_n(\mathbf{r}) \tag{2.3.S.11}$$

Now use,

$$\mathbb{D}G(\mathbf{r}, \mathbf{r}') = -4\pi\delta(\mathbf{r} - \mathbf{r}') \tag{2.3.S.12}$$

Since $\mathbb{D}$ is a linear operator,

$$\mathbb{D}G(\mathbf{r}, \mathbf{r}') = \sum_n a_n \mathbb{D}\psi_n(\mathbf{r}) = \sum_n a_n \lambda_n \psi_n(\mathbf{r}) = -4\pi\delta(\mathbf{r} - \mathbf{r}') = -4\pi \sum_n \psi_n^*(\mathbf{r}')\psi_n(\mathbf{r}) \tag{2.3.S.13}$$

$$\Rightarrow \quad \sum_n \left[a_n \lambda_n + 4\pi\psi_n^*(\mathbf{r}')\right] \psi_n(\mathbf{r}) = 0 \tag{2.3.S.14}$$

If a series in a set of basis functions vanishes, then each coefficient in the series must vanish, so,

$$\Rightarrow \quad a_n = -\frac{4\pi\psi_n^*(\mathbf{r}')}{\lambda_n} \tag{2.3.S.15}$$

from which we have,

$$\boxed{G(\mathbf{r}, \mathbf{r}') = -4\pi \sum_n \frac{\psi_n^*(\mathbf{r}')\psi_n(\mathbf{r})}{\lambda_n}} \tag{2.3.S.16}$$

<u>Example</u>

Consider the operator ∇^2 in rectangular coordinates, V is all of space. The eigenvalue problem is

$$\nabla^2\psi(\mathbf{r}) = \lambda\psi(\mathbf{r}) \tag{2.3.S.17}$$

Call the eigenvalues $\lambda = -k^2$. The eigenfunctions are then $\psi \sim \mathrm{e}^{i\mathbf{k}\cdot\mathbf{r}}$.

[Check: $\boldsymbol{\nabla}\psi = i\mathbf{k}\mathrm{e}^{i\mathbf{k}\cdot\mathbf{r}}$, so $\nabla^2\psi = \boldsymbol{\nabla}\cdot(\boldsymbol{\nabla}\psi) = (i\mathbf{k})\cdot(i\mathbf{k})\mathrm{e}^{i\mathbf{k}\cdot\mathbf{r}} = -k^2\psi$]

Normalize ψ for orthogonality condition. If we take $\psi_{\mathbf{k}}(\mathbf{r}) = \frac{1}{(2\pi)^{3/2}}\mathrm{e}^{i\mathbf{k}\cdot\mathbf{r}}$, then

$$\int d^3r\, \psi_{\mathbf{k}'}^*(\mathbf{r})\psi_{\mathbf{k}}(\mathbf{r}) = \int d^3r\, \frac{1}{(2\pi)^3}\mathrm{e}^{-i\mathbf{k}'\cdot\mathbf{r}}\mathrm{e}^{i\mathbf{k}\cdot\mathbf{r}} = \int d^3r\, \frac{\mathrm{e}^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}}}{(2\pi)^3} = \delta(\mathbf{k} - \mathbf{k}') \tag{2.3.S.18}$$

So,

$$G(\mathbf{r}, \mathbf{r}') = -4\pi \int \frac{d^3k}{(2\pi)^3}\, \frac{\mathrm{e}^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')}}{-k^2} = \int \frac{d^3k}{(2\pi)^3} \left(\frac{4\pi}{k^2}\right) \mathrm{e}^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r})} \tag{2.3.S.19}$$

Now we already know that the Green's function for ∇^2 is,

$$G(\mathbf{r}, \mathbf{r}') = \frac{1}{|\mathbf{r} - \mathbf{r}'|} \tag{2.3.S.20}$$

so from this we see that the Fourier transform of $\dfrac{1}{|\mathbf{r}|}$ is $\dfrac{4\pi}{k^2}$, something we have already found in Notes 1-5.

<u>Example</u>

Now consider the Green's function for ∇^2, but inside a rectangular box and satisfying the Dirichlet boundary condition on the surface of the box. The volume of the box is $x \in [0, a]$, $b \in [0, b]$, and $z \in [0, c]$.

We are looking for the eigenfunction of

$$\nabla^2 \psi = \lambda \psi \tag{2.3.S.21}$$

with $\psi = 0$ on the boundaries of the rectangular box.

The solutions are,

$$\psi_{\ell mn} = \sqrt{\frac{8}{abc}} \sin\left(\frac{\ell \pi x}{a}\right) \sin\left(\frac{m\pi y}{b}\right) \sin\left(\frac{n\pi z}{c}\right) \tag{2.3.S.22}$$

with eigenvalues

$$\lambda_{\ell mn} = -\pi^2 \left(\frac{\ell^2}{a^2} + \frac{m^2}{b^2} + \frac{n^2}{c^2}\right) \quad \text{with} \quad \ell, m, n = 1, 2, \ldots \quad \text{integers} \tag{2.3.S.23}$$

[Check the normalization is correct for yourselves!]

So we can now construct the Green's function,

$$G(\mathbf{r}, \mathbf{r}') = -4\pi \sum_{\ell,m,n=1}^{\infty} \frac{8}{abc} \frac{\sin\left(\frac{\ell\pi x}{a}\right) \sin\left(\frac{\ell\pi x'}{a}\right) \sin\left(\frac{m\pi y}{b}\right) \sin\left(\frac{m\pi y'}{b}\right) \sin\left(\frac{n\pi z}{c}\right) \sin\left(\frac{n\pi z'}{c}\right)}{-\pi^2 \left(\frac{\ell^2}{a^2} + \frac{m^2}{b^2} + \frac{n^2}{c^2}\right)} \tag{2.3.S.24}$$

$$= \frac{32}{\pi abc} \sum_{\ell,m,n=1}^{\infty} \frac{\sin\left(\frac{\ell\pi x}{a}\right) \sin\left(\frac{\ell\pi x'}{a}\right) \sin\left(\frac{m\pi y}{b}\right) \sin\left(\frac{m\pi y'}{b}\right) \sin\left(\frac{n\pi z}{c}\right) \sin\left(\frac{n\pi z'}{c}\right)}{\left(\frac{\ell^2}{a^2} + \frac{m^2}{b^2} + \frac{n^2}{c^2}\right)} \tag{2.3.S.25}$$

Note that in this case, $G(\mathbf{r}, \mathbf{r}')$ is *not* a function of $\mathbf{r} - \mathbf{r}'$. The boundary breaks the translational invariance.