Eigenfunction expansion for Green Functions

Suppose $\mathbb{D}$ is some <u>linear</u> differential operator, for example ∇^2.

Solutions to the equation

$$\mathbb{D}\,\psi(\vec{r}) = -4\pi f(\vec{r})$$

can be solved if one knows the Green function, which is the solution to the problem with a point source

$$\mathbb{D}\,G(\vec{r},\vec{r}\,') = -4\pi\,\delta(\vec{r}-\vec{r}\,')$$

operates on $\vec{r}$

Then

$$\psi(\vec{r}) = \int d^3r'\, G(\vec{r},\vec{r}\,')\, f(\vec{r}\,') \qquad \text{is solution}$$

If we need to solve for ψ subject to certain boundary conditions, then we can always add to the Green function a $\Phi(\vec{r})$ such that $\mathbb{D}\Phi(\vec{r}) = 0$ in the desired region and then choose Φ accordingly as we did for Dirichlet or Neumann b.c. for ∇^2.

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

$$\mathbb{D}\,\psi_n(\vec{r}) = \lambda_n \psi_n(r)$$

eigenfunction — eigenvalue

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 method, what we wound up doing was solving the eigen value problem for the (in spherical case) radial, θ, and φ pieces of the differential operator.]

In many cases (you would have to prove this for the particular operator $\mathbb{D}$) the eigen functions $\psi_n(\vec{r})$ form an <u>orthogonal</u> and <u>complete</u> <u>set of basis functions</u> over the region of interest (ie in the volume in which we are seeking a solution)

<u>orthogonal</u> $\Rightarrow$ $$\boxed{\int_V d^3r \; \psi_m^*(\vec{r})\,\psi_n(\vec{r}) = \delta_{m,n}}$$

<u>complete</u> $\Rightarrow$ $$f(\vec{r}) = \sum_n a_n \psi_n(\vec{r})$$

any function f can be expanded in a linear combination of the ψ_n.

The expansion coefficients a_n are obtained by

$$\int_V d^3r \; f(\vec{r})\,\psi_m^*(\vec{r}) = \sum_n a_n \int_V d^3r \; \psi_m^*(\vec{r})\,\psi_n(\vec{r}) = \sum_n a_n \delta_{m,n}$$

So $$\boxed{a_m = \int_V d^3r \; f(\vec{r})\,\psi_m^*(\vec{r})}$$ "Fourier" coefficient for basis ψ_n

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

$$\delta(\vec{r}-\vec{r}\,') = \sum_n a_n \psi_n(\vec{r})$$

where

$$a_n = \int_V d^3r\ \delta(\vec{r}-\vec{r}\,')\,\psi_n^*(\vec{r}) = \psi_n^*(\vec{r}\,') \quad \text{assuming } \vec{r}\,' \in V$$

So we have $\boxed{\delta(\vec{r}-\vec{r}\,') = \sum_n \psi_n^*(\vec{r}\,')\psi_n(\vec{r})}$

Now we can solve for the Green function!

Expand $G(\vec{r},\vec{r}\,')$ as, a function of $\vec{r}$, in a series in $\psi_n(\vec{r})$

$$G(\vec{r},\vec{r}\,') = \sum_n a_n \psi_n(\vec{r})$$

Now use

$$\mathbb{D}G(\vec{r},\vec{r}\,') = -4\pi\,\delta(\vec{r}-\vec{r}\,')$$

since $\mathbb{D}$ is linear

$$\hookrightarrow \sum_n a_n \mathbb{D}\psi_n(\vec{r}) = \sum_n a_n \lambda_n \psi_n(\vec{r}) = -4\pi \sum_n \psi_n^*(\vec{r}\,')\psi_n(\vec{r})$$

$$\Rightarrow \sum_n \left[a_n \lambda_n + 4\pi\,\psi_n^*(\vec{r}\,') \right] \psi_n(\vec{r}) = 0$$

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

$$\Rightarrow \quad a_n = -\frac{4\pi\,\psi_n^*(\vec{r}\,')}{\lambda_n}$$

$$\boxed{G(\vec{r},\vec{r}\,') = -4\pi \sum_n \left[\frac{\psi_n^*(\vec{r}\,')\psi_n(\vec{r})}{\lambda_n}\right]}$$

Example: ∇^2 in rectangular coordinate, V = all space

$$\nabla^2 \psi(\vec{r}) = \lambda \psi(\vec{r})$$

call the eigenvalues $\lambda = -k^2$

eigen functions are then $\psi \sim e^{i\vec{k}\cdot\vec{r}}$

check $\vec{\nabla}\psi = i\vec{k}\, e^{i\vec{k}\cdot\vec{r}}$

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

normalize ψ for orthogonality condition $\boxed{\psi_k(\vec{r}) = \frac{1}{(2\pi)^{3/2}} e^{i\vec{k}\cdot\vec{r}}}$

$$\int d^3r\, \psi^*_{k'}(\vec{r})\, \psi_k(\vec{r}) = \int d^3r \frac{1}{(2\pi)} e^{-i\vec{k}'\cdot\vec{r}} e^{i\vec{k}\cdot\vec{r}}$$

$$= \int d^3r \frac{e^{i(\vec{k}-\vec{k}')\cdot\vec{r}}}{(2\pi)^3} = \delta(\vec{k}-\vec{k}')$$

$$\Rightarrow \quad G(\vec{r},\vec{r}') = -4\pi \int \frac{d^2k}{(2\pi)^3} \frac{e^{i\vec{k}\cdot(\vec{r}-\vec{r}')}}{(-k^2)} = \int \frac{d^3k}{(2\pi)^3} \left(\frac{4\pi}{k^2}\right) e^{i\vec{k}\cdot(\vec{r}-\vec{r}')}$$

Now we already know that the Green function for this problem is

$$G(\vec{r},\vec{r}') = \frac{1}{|\vec{r}-\vec{r}'|}$$

So from this we see that the Fourier transf of

$$\frac{1}{|\vec{r}-\vec{r}'|} \text{ is } \frac{4\pi}{k^2}$$

Example Green's function for Dirichlet problem inside rectangular box $x \in [0, a]$, $y \in [0, b]$, $z \in [0, c]$

We are looking for eigenfunction of

$$\nabla^2 \psi = \lambda \psi$$

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

Solutions are

$$\psi_{lmn} = \sqrt{\frac{8}{abc}} \sin\left(\frac{l\pi x}{a}\right) \sin\left(\frac{m\pi y}{b}\right) \sin\left(\frac{n\pi z}{c}\right)$$

with eigenvalue $\lambda_{lmn} = -\pi^2\left(\frac{l^2}{a^2} + \frac{m^2}{b^2} + \frac{n^2}{c^2}\right)$, $lmn = 1, \ldots \infty$

check normalization for yourselves!

$$G(\vec{r}, \vec{r}') = -4\pi \sum_{lmn=1}^{\infty} \frac{8}{abc} \frac{\sin\left(\frac{l\pi x}{a}\right) \sin\left(\frac{l\pi x'}{a}\right) \sin\left(\frac{m\pi y}{b}\right) \sin\left(\frac{m\pi y'}{b}\right) \times \sin\left(\frac{n\pi z}{c}\right) \sin\left(\frac{n\pi z'}{c}\right)}{-\pi^2\left(\frac{l^2}{a^2} + \frac{m^2}{b^2} + \frac{n^2}{c^2}\right)}$$

$$G(\vec{r}, \vec{r}') = \frac{32}{\pi abc} \sum_{lmn=1}^{\infty} \frac{\sin\left(\frac{l\pi x}{a}\right) \sin\left(\frac{l\pi x'}{a}\right) \sin\left(\frac{m\pi y}{b}\right) \sin\left(\frac{m\pi y'}{b}\right) \sin\left(\frac{n\pi z}{c}\right) \sin\left(\frac{n\pi z'}{c}\right)}{\left(\frac{l^2}{a^2} + \frac{m^2}{b^2} + \frac{n^2}{c^2}\right)}$$

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