Eigenfunction Expansions of Green Functions

"Quantum meets E+M"

Another technique for obtaining Green functions is to use the eigenfunctions of a related problem.
Goal: Expand a Green function in terms of the eigenfunctions of the underlying problem.

$\mathcal{L}$: linear differential operator

Consider a linear differential operator: $\mathcal{L}\, u(\vec{x}) = \lambda\, u(\vec{x})$ [general eigenvalue problem]
on a region Ω

λ: eigenvalue

$\mathcal{L}$ said to be Hermitian if:

$$\underbrace{\int_\Omega u^*(\vec{x})\,\mathcal{L}\,v(\vec{x})\,d^3x}_{} = \left[\int_\Omega v^*(\vec{x})\,\mathcal{L}\,u(\vec{x})\,d^3x\right]^* = \int_\Omega v\,\mathcal{L}\,u^*\,d^3x$$

u, v : arbitrary functions obeying the boundary condition(s)

("u, v matrix element of $\mathcal{L}$") = ("v, u matrix element of $\mathcal{L}$")*

Now take $\mathcal{L}$ to be Hermitian. Consider particular eigenvalue λ_i and its eigenfunction $u_i(\vec{x}) \Rightarrow \mathcal{L}u_i(\vec{x}) = \lambda_i u_i(\vec{x})$
and another: λ_j ...... $u_j(\vec{x}) \Rightarrow \mathcal{L}u_j(\vec{x}) = \lambda_j u_j(\vec{x})$

So from this it follows trivially that:

① $$\int_\Omega d^3x\, u_j^*(\vec{x})\,\mathcal{L}\,u_i(\vec{x}) = \lambda_i \int_\Omega d^3x\, u_j^*(\vec{x})\, u_i(\vec{x})$$

② $$\underbrace{\int_\Omega d^3x\, u_i^*(\vec{x})\,\mathcal{L}\,u_j(\vec{x})}_{} = \lambda_j \int_\Omega d^3x\, u_i^*(\vec{x})\, u_j(\vec{x})$$

Look on left-hand side. Since $\mathcal{L}$ is, by assumption, Hermitian, it must be that

[LHS of ①] = [LHS of ②]*

by definition of ~~Hermitian $\mathcal{L}$~~ above

$\Longrightarrow$ applying this to RHS

$\Rightarrow$ RHS of ① = [RHS of ②]*

$$\lambda_i \int_\Omega d^3x\, u_j^*(\vec{x})\, u_i(\vec{x}) = \lambda_j^* \int_\Omega d^3x\, u_i^*(\vec{x})\, u_j(\vec{x})$$

$$\Rightarrow (\lambda_i - \lambda_j^*) \int_\Omega d^3x\, u_i(\vec{x})\, u_j^*(\vec{x}) = 0$$

From this, we see the results familiar to us from quantum mechanics for a Hermitian operator:

① eigenvalues are real [if $i=j$, must have $\lambda_i = \lambda_i^*$ to satisfy this equation]

② if $i \neq j$, $\lambda_i \neq \lambda_j \Rightarrow \int_\Omega d^3x\, u_i(\vec{x})\, u_j^*(\vec{x}) = 0 \Longrightarrow$ eigenfunctions of Hermitian operator are orthogonal (easy to make $\to$ orthonormal)

Now let us consider the inhomogeneous equation: $\mathcal{L}\psi(\vec{x}) - \lambda\psi(\vec{x}) = f(\vec{x})$ on domain Ω

$\mathcal{L}$: Hermitian differential operator

$\psi(\vec{x})$ s.t. b.c.'s on Ω

λ: some given constant; in general, not necessarily an eigenvalue of $\mathcal{L}$

__To solve:__ expand $\psi(\vec{x})$ and $f(\vec{x})$ in terms of eigenfunctions of $\mathcal{L}$! (the $u_n(\vec{x})$)

$$\psi(\vec{x}) = \sum_n c_n u_n(\vec{x}) \qquad f(\vec{x}) = \sum_n d_n u_n(\vec{x})$$

[makes sense, can then match coefficients to solve the equation

Substituting into the above gives:

$$\sum_n c_n \underbrace{\mathcal{L} u_n(\vec{x})} - \lambda \sum_n c_n u_n(\vec{x}) = \sum_n d_n u_n(\vec{x})$$

$$\sum_n \left(c_n \lambda_n u_n(\vec{x}) - \lambda c_n u_n(\vec{x}) \right) = \sum_n \left(d_n u_n(\vec{x}) \right)$$

$$\Rightarrow \quad c_n \lambda_n - \lambda c_n = d_n \Rightarrow c_n = \frac{d_n}{\lambda_n - \lambda}$$

matching the $u_n(\vec{x})$ terms

But, recall in general we can write: $f(\vec{x}) = \sum_n d_n u_n(\vec{x}) \Rightarrow \int_\Omega d^3x\, u_n^*(\vec{x}) f(\vec{x}) = d_n$

$$\Rightarrow c_n = \frac{\int_\Omega d^3x\, u_n^*(\vec{x}) f(\vec{x})}{\lambda_n - \lambda}$$

Thus, we can write:

$$\psi(\vec{x}) = \sum_n c_n u_n(\vec{x}) = \sum_n u_n(\vec{x}) \cdot \left[\frac{\int_\Omega d^3x\, u_n^*(\vec{x}) f(\vec{x})}{\lambda_n - \lambda} \right]$$

$$= \sum_n \frac{u_n(\vec{x})}{\lambda_n - \lambda} \left[\int_\Omega d^3x\, u_n^*(\vec{x}) f(\vec{x}) \right]$$

clearly Hermitian, as we know from Quantum Mechanics! [Schrödinger Eq.]

Now, if we let: $\mathcal{L} = \vec{\nabla}^2$, $\psi = G(\vec{x}, \vec{x}')$, $f(\vec{x}) = -4\pi\,\delta(\vec{x}-\vec{x}')$, $\lambda = 0$:

$$\vec{\nabla}^2 G(\vec{x},\vec{x}') = -4\pi\,\delta(\vec{x}-\vec{x}')$$ [familiar equation defining the Green function]

Therefore $\Rightarrow$ we can write:

$$\underline{\underline{G(\vec{x},\vec{x}')}} = \sum_n \frac{\overbrace{u_n(\vec{x})}^{\text{eigenfunctions of } \mathcal{L}=\vec{\nabla}^2 \text{ s.t. boundary conditions!}}}{\lambda_n - 0}\left[\int_\Omega d^3x\; u_n^*(\vec{x})\overbrace{(-4\pi)\,\delta(\vec{x}-\vec{x}')}^{f(\vec{x}) = -4\pi\,\delta(\vec{x}-\vec{x}')}\right]$$

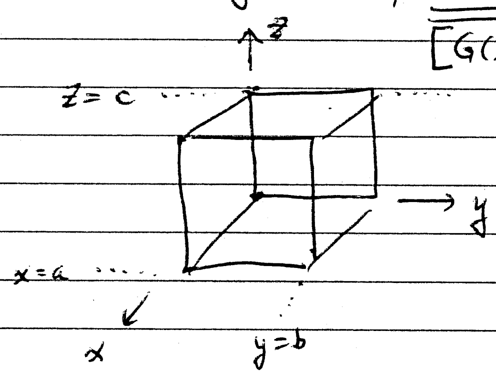
$$= -4\pi \sum_n \frac{u_n(\vec{x})}{\lambda_n}\underbrace{\int_\Omega d^3x\; u_n^*(\vec{x})\,\delta(\vec{x}-\vec{x}')}_{\text{so if } \vec{x}' \text{ in } \Omega \text{ (i.e., sources indeed in domain } \Omega)}$$

$$= \underline{\underline{-4\pi \sum_n \frac{u_n(\vec{x})\,u_n^*(\vec{x}')}{\lambda_n}}}$$

THIS IS AN EXPANSION of the Green Function $G(\vec{x},\vec{x}')$ in terms of the eigenfunctions $u_n(\vec{x})$ of the Hermitian operator $\vec{\nabla}^2$!

<u>Example</u>: Consider rectangular box, <u>Dirichlet problem</u>. Find the Green function!

[$G(\vec{x},\vec{x}') = 0$ on Surface]



So, from above:

$$G(\vec{x},\vec{x}') = -4\pi \sum_n \frac{u_n(\vec{x})\,u_n^*(\vec{x}')}{\lambda_n}$$

u_n are eigenfunctions of $\vec{\nabla}^2$ for the box! geometry

λ_n are eigenvalues: which satisfy the b.c.

$$\vec{\nabla}^2 u_n(\vec{x}) = \lambda_n u_n(\vec{x}) \quad \text{with } u_n(\vec{x}) = 0 \text{ on Surfaces}$$

$u_{lmn}(\vec{x}) \propto$

Clearly, suitable choices are: $\sin\left(\frac{l\pi x}{a}\right)\sin\left(\frac{m\pi y}{b}\right)\sin\left(\frac{n\pi z}{c}\right) \Rightarrow$ satisfies $u_{lmn} = 0$ on all surfaces

$$\vec{\nabla}^2 u_{lmn} = \left(-\frac{l^2\pi^2}{a^2} - \frac{m^2\pi^2}{b^2} - \frac{n^2\pi^2}{c^2}\right)\sin\left(\frac{l\pi x}{a}\right)\sin\left(\frac{m\pi y}{b}\right)\sin\left(\frac{n\pi z}{c}\right) = \lambda_{lmn}\sin\left(\frac{l\pi x}{a}\right)\sin\left(\frac{m\pi y}{b}\right)\sin\left(\frac{n\pi z}{c}\right)$$

$$\Rightarrow \lambda_{lmn} = -\pi^2\left(\frac{l^2}{a^2} + \frac{m^2}{b^2} + \frac{n^2}{c^2}\right)$$

Finally,

u_{lmn} must be orthonormal: (on domain Ω) $\Rightarrow$ let $u_{lmn} = \overset{\downarrow \text{normalization}}{N_x} \sin(\ldots x) \overset{N_y}{\sin}(\ldots y) \overset{N_z}{\sin}(\ldots z)$

$$\text{e.g.,}\quad \underset{\nearrow\,(\text{normalization})^2}{N_x^2} \int_0^a dx \cdot \sin^2\left(\frac{l\pi x}{a}\right) = N_x^2 \int_0^\pi \frac{a}{\pi}\, du \, \sin^2(lu) = \frac{N_x^2}{2} \frac{a}{\pi} \underbrace{\int_{-\pi}^{+\pi} du \, \sin(lu) \sin(lu)}_{= \pi \delta_{ll}}$$

$$\left[u = \frac{\pi x}{a}\right] \qquad du = \frac{\pi}{a} dx$$

$$= \frac{N_x^2}{2} \cdot \frac{a}{\pi} \cdot \pi \overset{(\text{must})}{=\!=} 1 \text{ for orthonorm.}$$

$$\Rightarrow N_x^2 = \frac{2}{a} \Rightarrow N_x = \sqrt{\frac{2}{a}}$$

$$\Rightarrow u_{lmn} = \sqrt{\frac{2}{a}} \sin\left(\frac{l\pi x}{a}\right) \sqrt{\frac{2}{b}} \sin\left(\frac{m\pi y}{b}\right) \sqrt{\frac{2}{c}} \sin\left(\frac{n\pi z}{c}\right)$$

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

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

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

✓