

Ch. 3.12 Eigenfunction Expansions for Green Functions

P.2

Let's consider a method to evaluate Green Functions that is alternative to the direct integration.

Consider an equation of the form

$$\nabla^2 \psi(\vec{x}) + [f(x) + \lambda] \psi(\vec{x}) = 0 \quad \text{in volume } V \quad (1)$$

where $\psi(\vec{x})$ has to satisfy the homogenous boundary conditions: Dirichlet, Neumann, $\psi(\vec{x})|_{\vec{x} \in S} = 0$

(Dirichlet)

$$\frac{\partial \psi}{\partial \vec{n}}(\vec{x})|_{\vec{x} \in S} = 0 \quad (\text{Neumann})$$

The solution of Eq. (1) exists only for certain values of λ , we call them λ_n , with n being an index numbering the eigenvalues:

$$\nabla^2 \psi_n(\vec{x}) + [f(\vec{x}) + \lambda_n] \psi_n(\vec{x}) = 0$$

Hence for each eigenvalue λ_n there is at least one eigenfunction $\psi_n(\vec{x})$

The eigenfunctions are orthogonal for different eigenvalues: consider $\lambda_n \neq \lambda_m$

$$\psi_m^*(\vec{x}) \nabla^2 \psi_n(\vec{x}) + \psi_m^*(\vec{x}) f(\vec{x}) \psi_n(\vec{x}) + \lambda_n \psi_m^*(\vec{x}) \psi_n(\vec{x}) = 0 \quad (2)$$

$$\psi_n^*(\vec{x}) \nabla^2 \psi_m(\vec{x}) + \psi_n^*(\vec{x}) f(\vec{x}) \psi_m(\vec{x}) + \lambda_m \psi_n^*(\vec{x}) \psi_m(\vec{x}) = 0 \quad (3)$$

Assuming $\lambda_m = \lambda_m^*$ take complex conjugated equation in a second line and subtract it from the first one:

$$\psi_m^*(\vec{x}) \nabla^2 \psi_n(\vec{x}) - \nabla^2 \psi_m^*(\vec{x}) \psi_n(\vec{x}) + (\lambda_n - \lambda_m) \psi_m^*(\vec{x}) \psi_n(\vec{x}) = 0$$

Integrate it over the volume V

From the Green's theorem

$$\int_V d^3x (\psi_m^*(\vec{x}) \nabla^2 \psi_n(\vec{x}) - \psi_n(\vec{x}) \nabla^2 \psi_m^*(\vec{x})) =$$

$$= \int_S d\vec{a} \cdot \vec{n} (\psi_m^*(\vec{x}) \nabla \psi_n(\vec{x}) - \psi_n(\vec{x}) \nabla \psi_m^*(\vec{x})) = 0$$

Thanks to the B.C. \nearrow

Remark: Strictly speaking we had to consider separately the real and imaginary parts of the above equation: the same argument then holds.

$$\lambda_n \neq \lambda_m \Rightarrow \int d^3x \psi_m^*(\vec{x}) \psi_n(\vec{x}) = 0$$

To show that $\lambda_n = \lambda_n^*$ just take $n=m$ in Eq.(3) and subtract it from (2)

$$\int_V d^3x (\psi_n^*(\vec{x}) \nabla^2 \psi_n(\vec{x}) - \psi_n(\vec{x}) \nabla^2 \psi_n^*(\vec{x})) +$$

$$+ (\lambda_n - \lambda_n^*) \int_V d^3x \psi_n^*(\vec{x}) \psi_n(\vec{x}) = 0$$

$$\Rightarrow \text{as } \int_V d^3x \psi_n^*(\vec{x}) \psi_n(\vec{x}) \neq 0 \Rightarrow \lambda_n = \lambda_n^*$$

We then get a normalized set of eigenfunctions

$$\int_V d^3x \psi_m^*(\vec{x}) \psi_n(\vec{x}) = \delta_{mn}$$

assumed to be complete, $\sum_n \psi_n^*(\vec{x}) \psi_n(\vec{x}') = \delta(\vec{x} - \vec{x}')$

Now solve for the Green function

$$\nabla_x^2 G(\vec{x}, \vec{x}') + [f(\vec{x}) + \lambda] G(\vec{x}, \vec{x}') = -4\pi \delta(\vec{x} - \vec{x}') \quad (4)$$

with Green function satisfying the same B.C.

Look for the solution in the form

(p.3)

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

(5)

Substitute (5) into (4) with $\lambda \neq \lambda_n \leftarrow$ important!

$$[\nabla_x^2 + f(x)] \sum_m a_m(\vec{x}') \psi_m(\vec{x}) + \lambda \sum_m a_m(\vec{x}') \psi_m(\vec{x}) = -4\pi \delta(\vec{x} - \vec{x}')$$

$$\Rightarrow \sum_m a_m(\vec{x}') (\lambda - \lambda_m) \psi_m(\vec{x}) = -4\pi \delta(\vec{x} - \vec{x}')$$

multiply by $\psi_n^*(\vec{x})$ and integrate over V

$$a_n(\vec{x}') (\lambda - \lambda_n) = -4\pi \psi_n^*(\vec{x}')$$

$$\Rightarrow a_n(\vec{x}') = 4\pi \frac{\psi_n^*(\vec{x}')}{\lambda_n - \lambda}$$

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

(6)

if the spectrum is continuous the sum is replaced by integral.

Consider the Poisson equation: $f(\vec{x})=0, \lambda=0$
 $\nabla^2 \psi = 0$

in a free space the eigenfunctions are labeled by the continuous index (vector) \vec{k}

$$\psi_{\vec{k}}(\vec{x}) = \frac{e^{i\vec{k} \cdot \vec{x}}}{(2\pi)^{3/2}}, \quad \int d^3x \psi_{\vec{k}'}^*(\vec{x}) \psi_{\vec{k}}(\vec{x}) = \delta(\vec{k} - \vec{k}')$$

$\lambda_{\vec{k}} = +|\vec{k}|^2$

Now the Green function $G(\vec{x}, \vec{x}') = \frac{1}{|\vec{x} - \vec{x}'|}$ satisfies

$$\nabla_x^2 G(\vec{x}, \vec{x}') = -4\pi \delta(\vec{x} - \vec{x}')$$

From Eq. (6)

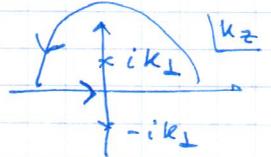
$$G(\vec{x}-\vec{x}') = \frac{1}{|\vec{x}-\vec{x}'|} = 4\pi \int \frac{d^3\vec{k}}{(2\pi)^3} \frac{e^{i\vec{k}(\vec{x}-\vec{x}')}}{k^2} =$$

$$= \frac{1}{2\pi^2} \int d^3k \frac{e^{i\vec{k}(\vec{x}-\vec{x}')}}{k^2}$$

Let's rewrite it slightly differently

$$G(\vec{x}-\vec{x}') = \frac{1}{2\pi^2} \int d^2k_{\perp} \int dk_z \frac{e^{ik_z(z-z')}}{k_z^2 + k_{\perp}^2} e^{i\vec{k}_{\perp} \cdot \vec{r}_{\perp}}, \quad \begin{matrix} \vec{r}_{\perp} \equiv (x, y) \\ \vec{k}_{\perp} \equiv (k_x, k_y) \end{matrix}$$

$z-z' > 0$



$$\Rightarrow \int dk_z \frac{e^{ik_z(z-z')}}{k_z^2 + k_{\perp}^2} =$$

$$= \oint dk_z \frac{e^{ik_z(z-z')}}{(k_z + ik_{\perp})(k_z - ik_{\perp})} = 2\pi i \frac{e^{-k_{\perp}(z-z')}}{2ik_{\perp}} =$$

$$= \frac{\pi}{k_{\perp}} e^{-k_{\perp}(z-z')}$$

As the above integral is symmetric with respect to $z-z' \rightarrow z'-z$ we finally obtain

$$G(\vec{x}-\vec{x}') = \frac{1}{2\pi} \int d^2k_{\perp} \frac{e^{i\vec{k}_{\perp} \cdot \vec{r}_{\perp}}}{k_{\perp}} e^{-k_{\perp}(z-z')}$$

which is Weyl's formula obtained earlier by the method of direct integration.

The second example: Dirichlet problem inside a rectangular box defined by six planes $x=0, y=0, z=0, x=a, y=b, z=c$

$$(\nabla^2 + k_{emn}^2) \psi_{emn} = 0$$

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

$$k_{emn}^2 = \pi^2 \left(\frac{l^2}{a^2} + \frac{m^2}{b^2} + \frac{n^2}{c^2} \right)$$

$$\Rightarrow G(\vec{x}, \vec{x}') = \frac{32}{\pi abc} \times$$

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

We could apply the method of direct integration by writing

$$\begin{aligned} \delta(\vec{x} - \vec{x}') &= \delta(x - x') \delta(y - y') \delta(z - z') = \\ &= \sqrt{\frac{4}{ab}} \left(\sum_{em} \sin\left(\frac{l\pi x}{a}\right) \sin\left(\frac{l\pi x'}{a}\right) \sin\left(\frac{m\pi y}{b}\right) \sin\left(\frac{m\pi y'}{b}\right) \right) \delta(z - z') \end{aligned}$$

$$\begin{aligned} G(\vec{x}, \vec{x}') &= \frac{16\pi}{ab} \sum_{em=1}^{\infty} \sin\left(\frac{l\pi x}{a}\right) \sin\left(\frac{l\pi x'}{a}\right) \sin\left(\frac{m\pi y}{b}\right) \sin\left(\frac{m\pi y'}{b}\right) \times \\ &\times \frac{\sinh(k_{em} z) \sinh[k_{em}(c - z)]}{k_{em} \sinh(k_{em} c)} \end{aligned}$$

$$k_{em} = \pi \left(\frac{l^2}{a^2} + \frac{m^2}{b^2} \right)^{1/2}$$

The two expressions are equivalent as

$$\frac{\sinh(k_{em} z) \sinh(k_{em}(c - z))}{k_{em} \sinh(k_{em} c)} = \frac{2}{c} \sum_{n=1}^{\infty} \frac{\sin\left(\frac{n\pi z'}{c}\right) \sin\left(\frac{n\pi z}{c}\right)}{k_{em}^2 + \left(\frac{n\pi}{c}\right)^2}$$

The RHS is Fourier transform of the LHS (Mathematica)