

Reciprocity relation for Green's function

$\hat{A}_{\vec{r}}$ is hermitian for domain D and corresponding B.C. if
 & u, v functions defined on D under the B.C.:

$$\langle u | \hat{A}_{\vec{r}} | v \rangle = \langle v | \hat{A}_{\vec{r}}^* | u \rangle^* \quad \text{where } \langle \vec{r} | u \rangle = u(\vec{r}) \\ \langle u | \vec{r} \rangle = u^*(\vec{r})$$

in terms of integrals, this is rewritten as

$$\int d\vec{r} u^*(\vec{r}) (\hat{A}_{\vec{r}} v(\vec{r})) = \left(\int d\vec{r} v^*(\vec{r}) \hat{A}_{\vec{r}} u(\vec{r}) \right)^* = \int d\vec{r} (\hat{A}_{\vec{r}} u(\vec{r}))^* v(\vec{r})$$

now take $u(\vec{r}) = G(\vec{r}, \vec{r}_2)$ and $v(\vec{r}) = G(\vec{r}, \vec{r}_1)$, for given \vec{r}_1, \vec{r}_2

$$\int d\vec{r} G^*(\vec{r}, \vec{r}_2) \underbrace{\hat{A}_{\vec{r}} G(\vec{r}, \vec{r}_1)}_{\delta(\vec{r} - \vec{r}_1)} = \int d\vec{r} \underbrace{(\hat{A}_{\vec{r}} G(\vec{r}, \vec{r}_2))^*}_{\delta(\vec{r} - \vec{r}_2)} G(\vec{r}, \vec{r}_1)$$

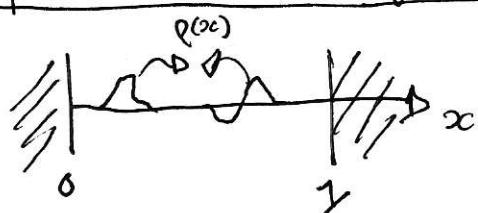
so

$$G^*(\vec{r}_1, \vec{r}_2) = G(\vec{r}_2, \vec{r}_1)$$

In the linear algebra point of view, this is the analog of

$$A^+ = A \Rightarrow \underbrace{(A^{-1})^+}_{G} = A^{-1} \text{ or } G^+ = G.$$

Example with boundary conditions



$$\frac{d^2\phi}{dx^2} + m^2 \phi = \rho(x) \text{ with } \phi(0) = \phi(1) = 0$$

1. homogeneous equation: (particle in a box or the tight rope problem)

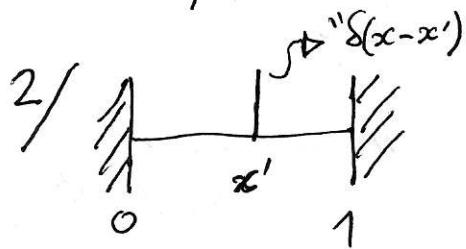
$$\frac{d^2\phi}{dx^2} + m^2 \phi = 0 \Rightarrow \boxed{\phi(x) = A \sin(mx) + B \cos(mx)}$$

$$\text{with } \phi(0) = \phi(1) = 0 \Rightarrow B = 0 \text{ and } \sin(m_n) = 0 \Rightarrow \boxed{m_n = n\pi} \quad \text{with } n = 1, 2, \dots$$

the functions are $\phi_n = A_n \sin(m_n x)$

$$\text{with } A_n = \sqrt{\frac{2}{l}} \text{ if we want the normalisation} \quad \boxed{\int_0^1 dx \phi_n^2(x) = 1}$$

let $\hat{A}_x = \frac{d^2}{dx^2} + m^2$ be the one dimensional Helmholtz operator:
 we see that $\hat{A}_x \phi_n = (-m_n^2 + m^2) \phi_n$ with the good B.C. for ϕ_n
 so the ϕ_n are the eigenstates of \hat{A}_x with eigenvalues $\lambda_n = m^2 - (n\pi)^2$



the delta function splits the problem in two homogeneous problems on $[0, x']$ and $[x', 1]$
 but we need to find the boundary conditions at $x=x'$, that is, we need to derive the continuity equations for $x=x'$ for $G(x, x')$

From the differential equation, we have. (x' a parameter):

$$G''(x, x') = -m^2 G(x, x') + \delta(x - x') \quad G'' \uparrow$$

so G'' is "delta" discontinuous at $x=x'$

$$\int_{x'-\epsilon}^{x'+\epsilon} G''(x, x') dx = G'(x'+\epsilon, x') - G'(x'-\epsilon, x') = -m^2 \int_{x'-\epsilon}^{x'+\epsilon} dx G(x, x') + 1 \quad \text{finite in the principal value sense}$$

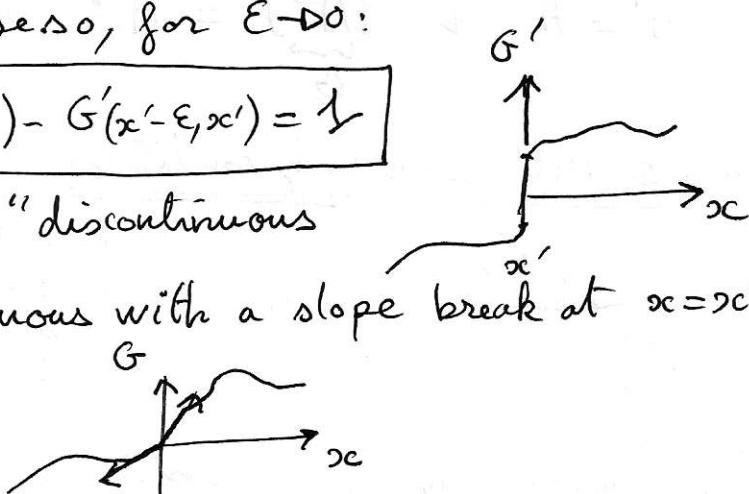
We assume that $G(x, x')$ is finite $\Delta \epsilon \rightarrow 0$

in the principal value sense so, for $\epsilon \rightarrow 0$:

$$\lim_{\epsilon \rightarrow 0} [G'(x'+\epsilon, x') - G'(x'-\epsilon, x')] = 1$$

so $G'(x, x')$ is "theta" discontinuous

and $G(x, x')$ is continuous with a slope break at $x=x'$



3/ Solution on $[0, x']$:

$$g_L(x) = A \sin(m x) \quad \text{since } g_L(0) = 0$$

Solution on $[x', 1]$:

$$g_R(x) = B \sin(m(1-x)) \quad \text{since } g_R(1) = 0$$

We must now connect the two solutions at $x=x'$:

$$\text{continuity: } g_L(x') = g_R(x') \Rightarrow A \sin(mx') = B \sin(m(1-x'))$$

$$\text{discontinuity: } g_R(x') = g_L(x') + 1 \Rightarrow -mB \cos(m(1-x')) = mA \cos(mx') + 1$$

$$\text{let us write } s = \sin(mx'), s' = \sin(m(1-x'))$$

$$c = \cos(mx'), c' = \cos(m(1-x'))$$

A and B are solutions of the linear system:

$$\begin{pmatrix} s & -s' \\ mc & mc' \end{pmatrix} \begin{pmatrix} A \\ B \end{pmatrix} = \begin{pmatrix} 0 \\ -1 \end{pmatrix}$$

which is invertible provided the determinant is non-zero

$$\begin{aligned} \det &= smc' + mcs' = m(\sin(mx')\cos(m(1-x')) + \cos(mx')\sin(m(1-x'))) \\ &= m \sin(mx' + m(1-x')) = m \sin(m) > 0 \end{aligned}$$

we thus assume that $m \neq n\pi$, $n \in \mathbb{N}$, i.e. that there is no zero eigenvalue in the spectrum of the operator.

We get

$$\begin{pmatrix} A \\ B \end{pmatrix} = \frac{1}{m \sin(m)} \begin{pmatrix} mc' & s' \\ -mc & s \end{pmatrix} \begin{pmatrix} 0 \\ -1 \end{pmatrix} \Rightarrow \begin{cases} A = -\frac{\sin(m(1-x'))}{m \sin(m)} \\ B = -\frac{\sin(mx')}{m \sin(m)} \end{cases}$$

and finally,

$$\boxed{\begin{aligned} g_L(x) &= \frac{\sin(mx)\sin(m(x-1))}{m \sin(m)} \\ g_R(x) &= \frac{\sin(m(x-1))\sin(mx)}{m \sin(m)} \end{aligned}}$$

4/ We have $\text{Tr}(\hat{A}_x^{-1}) = \text{Tr}(\hat{G}) = \int_0^1 dx G(x, x) = \sum_{n=1}^{\infty} \frac{1}{\lambda_n} = \sum_{n=1}^{\infty} \frac{1}{m^2(n\pi)^2}$

but $\int_0^1 dx \frac{\sin(mx)\sin(m(x-1))}{m \sin(m)} = \frac{1}{m \sin(m)} \int_0^1 dx \left[\underbrace{\cos(mx - m(x-1))}_{\cos(m)} - \underbrace{\cos(mx + m(x-1))}_{\cos(2mx-m)} \right]$

$$= \frac{1}{2m \sin(m)} \left[\cos(m) - \left[\underbrace{\frac{\sin(2mx-m)}{2m}}_0 \right] \right]$$

$$= \frac{1}{2m \sin(m)} (\sin(m) - (-\sin(m))) = \frac{\sin(m)}{m}$$

$$\text{Thus, } \sum_{n=1}^{\infty} \frac{1}{m^2 - (n\pi)^2} = \frac{1}{2m} \left[\cot(m) - \frac{1}{m} \right] \text{ or}$$

$$\cot(m) = \frac{1}{m} + \sum_{n=1}^{\infty} \frac{2m}{m^2 - (n\pi)^2}$$

Diffusion equation

We have $\left(\frac{\partial}{\partial t} - D\Delta \right) \phi(\vec{r}, t) = S(\vec{r}, t)$ with $\phi(\vec{r}, t) \xrightarrow[\vec{r} \rightarrow \infty]{ } 0 \forall t$
+ causality.

we move to Fourier space for the Green function

$$\left(\frac{\partial}{\partial t} - D\Delta_{\vec{r}} \right) G(\vec{r}, \vec{r}', t, t') = \delta(\vec{r} - \vec{r}') \delta(t - t')$$

$$\tilde{G}(\vec{k}, \vec{r}', \omega, t') = \int d\vec{r} \int dt e^{-i(\vec{k} \cdot \vec{r} - \omega t)} G(\vec{r}, \vec{r}', t, t')$$

$$\Rightarrow [i\omega - D(-\vec{k}^2)] \tilde{G} = e^{-i\vec{k} \cdot \vec{r}'} e^{i\omega t'}$$

$$\Rightarrow G(\vec{r}, \vec{r}', t, t') = \int \frac{d\vec{k}}{(2\pi)^3} \int \frac{d\omega}{2\pi} \frac{e^{i(\vec{k} \cdot \vec{r} - \omega t)} e^{-i\vec{k} \cdot \vec{r}'} e^{i\omega t'}}{-i\omega + D\vec{k}^2}$$

$$= \frac{1}{(2\pi)^4} \int d\vec{k} \int d\omega \frac{e^{i[\vec{k} \cdot (\vec{r} - \vec{r}') - \omega(t - t')]}}{-i\omega + D\vec{k}^2} ; \begin{matrix} \vec{z} = t - t' \\ \vec{d} = \vec{r} - \vec{r}' \end{matrix}$$

First, the integral over ω , we set $\omega_k = -iD\vec{k}^2 \Rightarrow$ on the imaginary axis

$$\int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} \frac{e^{-i\omega z}}{\omega - \omega_k} = \begin{cases} 0 & \text{if } z < 0 \\ \text{Causality!} & \end{cases}$$

index ↴

$$\underset{1.2\pi}{\frac{2i\pi(-1)}{1.2\pi}} \frac{e^{-i\omega_k z}}{1.2\pi} = -i e^{-D\vec{k}^2 z}$$

$$\therefore G(\vec{d}, z) = \frac{\Theta(z)}{(2\pi)^3} \int d\vec{k} \underbrace{i(-i)}_{\sigma_k^2 = \frac{1}{2Dz}} e^{-Dz\vec{k}^2} e^{i\vec{k} \cdot \vec{d}} = \Theta(z) \frac{1}{(2\pi \frac{1}{\sigma_k^2})^{3/2}} e^{-\frac{\vec{d}^2}{2\sigma_k^2}}$$

↑ Gaussian integrals

$$G(\vec{d}, z) = \Theta(z) \frac{1}{(4\pi Dz)^{3/2}} e^{-\vec{d}^2/4Dz}$$