Green's Functions

Example: $\vec{\nabla}\cdot\vec{E} = 4\pi\rho$ $\vec{E} = -\vec{\nabla}\phi - \frac{1}{c}\frac{\partial\vec{A}}{\partial t}$

In Coulomb gauge, $\nabla\cdot A = 0$, so there

$$-\Delta\phi = -\nabla^2\phi = 4\pi\rho.$$

Suppose we have a Green's function such that

$$-\nabla_1^2 G(x_1, x_2) = \delta^3(\vec{x}_1 - \vec{x}_2)$$

in fact

$$G(\vec{x}_1, \vec{x}_2) = G(\vec{x}_1 - \vec{x}_2) \quad \text{so}$$

$$-\nabla^2 G(\vec{x}) = \delta^{(3)}(\vec{x})$$

Then by Green's theorem with $\phi(x)$ and $G(\vec{x}-\vec{x}')$

$$\int(\phi\,\nabla^2 G - G\,\nabla^2\phi)\,d^3x = \int(\phi\vec{\nabla}G - G\vec{\nabla}\phi)\cdot d\vec{\sigma}$$

And if we assume that ϕ and G fall off suitably as $r\to\infty$ and also extend the volume integral over all of space, pushing the surface integral to infinity, then the surface integral vanishes, and we get

$$-\int\phi(\vec{x})\,\nabla^2 G(\vec{x}-\vec{x}')\,d^3x = -\int G(\vec{x}-\vec{x}')\nabla^2\phi(x)\,d^3x$$

$$\int\phi(\vec{x})\,\delta(x-x')\,d^3x = \phi(\vec{x}') \;=\!=\; \int G(\vec{x}-\vec{x}')\,4\pi\rho(x)\,d^3x$$

Letting $x \to x'$ and $x' \to x$, we get

$$\phi(\vec{x}) = \int G(\vec{x}' - \vec{x})\, 4\pi \rho(\vec{x}')\, d^3x' .$$

In fact, since G is defined by

$$-\nabla_1^2 G(x_1, x_2) = -\nabla_1^2 G(x_1 - x_2) = \delta^3(x_1 - x_2)$$

$$= \delta^3(x_2 - x_1) = -\nabla_2^2 G(x_2 - x_1)$$

$$= -\nabla_1^2 G(x_2 - x_1) = -\nabla_1^2 G(x_2, x_1)$$

we see that this Green's function is symmetric.

$$G(x_1, x_2) = G(x_2, x_1).$$

It's easy to find $G(\vec{x})$ such that

$$-\nabla^2 G(\vec{x}) = \delta^3(\vec{x})$$

Let $\displaystyle G(\vec{x}) = \int \frac{d^3k}{(2\pi)^3}\, e^{i\vec{k}\cdot\vec{x}}\, g(\vec{k})$ Then we want

$$-\nabla^2 G(\vec{x}) = \int \frac{d^3k}{(2\pi)^3}\, e^{i\vec{k}\cdot\vec{x}}\, \vec{k}^2 g(\vec{k}) = \int \frac{d^3k}{(2\pi)^3}\, e^{i\vec{k}\cdot\vec{x}} = \delta^3(\vec{x})$$

So $g(\vec{k}) = 1/\vec{k}^2$, and

$$G(\vec{x}) = \int \frac{d^3k}{(2\pi)^3}\, e^{i\vec{k}\cdot\vec{x}}\, \frac{1}{\vec{k}^2} = \int_{-1}^{1} d\mu \int_0^\infty \frac{k^2 dk}{(2\pi)^2}\, e^{ikr\mu}\, \frac{1}{k^2}$$

So

$$G(\vec{x}) = G(r) = \int_0^\infty \frac{dk}{(2\pi)^2} \, \frac{e^{ikr} - e^{-ikr}}{ikr}$$

$$= \frac{1}{r} \, \frac{1}{i} \frac{1}{(2\pi)^2} \int_{-\infty}^{\infty} dk \, \frac{e^{ikr}}{k}$$

$$= \frac{1}{2\pi r} \, \frac{1}{2\pi i} \, P \int_{-\infty}^{\infty} \frac{dz}{z} \, e^{iz}$$

$$\frac{1}{2\pi i} \, P \int_{-\infty}^{\infty} \frac{dz}{z} \, e^{iz} = \frac{1}{2\pi i} \int \frac{dz}{z} \, e^{iz} - \frac{1}{2\pi i} \int_{\frown} \frac{dz}{z} \, e^{iz}$$

$$= \frac{1}{2\pi i} \int_{\frown} \frac{dz}{z} \, e^{iz} = \frac{\pi i}{2\pi i} = \frac{1}{2}$$ so

$$G(\vec{x}) = \frac{1}{4\pi r}$$ or

$$G(x_1, x_2) = \frac{1}{4\pi \, |\vec{x}_1 - \vec{x}_2|} = G(x_2, x_1).$$

$$-\nabla_1^2 \, G(x_1, x_2) = \delta^3(x_1 - x_2)$$

$$= -\nabla_2^2 \, G(x_1, x_2).$$

So as we saw weeks ago

$$\phi(\vec{x}, t) = \int G(x - x')\, 4\pi \rho(x', t)\, d^3x'$$

$$= \int \frac{\rho(x', t)}{|\vec{x}' - \vec{x}'|}\, d^3x'$$

in the Coulomb gauge — and also in electrostatics in all gauges.

For the Helmholtz operator

$$(-\nabla^2 - k^2)\, G_H(x_1, x_2) = \delta^3(x_1 - x_2)$$

$$G_H(\vec{x}_1, \vec{x}_2) = \frac{\exp\left(ik\, |\vec{x}_1 - \vec{x}_2|\right)}{4\pi\, |\vec{x}_1 - \vec{x}_2|}$$

and for

$$(-\nabla^2 + k^2)\, G_{MH}(x_1, x_2) = \delta^3(\overrightarrow{x_1 - x_2}),$$

we get

$$G_{MH}(\vec{x}_1, \vec{x}_2) = \frac{\exp\left(-k\, |\overrightarrow{x_1 - x_2}|\right)}{4\pi\, |\vec{x}_1 - \vec{x}_2|}$$

both symmetric under $x_1 \rightleftarrows x_2$.

The spherical-harmonic expansion of the electrostatic Green's function is

$$G(\vec{x}_1, \vec{x}_2) = \frac{1}{4\pi |\vec{x}_1 - \vec{x}_2|}$$

$$= \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} \frac{1}{2\ell+1} \frac{r_<^{\ell}}{r_>^{\ell+1}} Y_\ell^m(\theta_1, \phi_1) Y_\ell^{m*}(\theta_2, \phi_2)$$

where

$$r_< = \begin{cases} |x_1| & \text{if } |x_1| < |x_2| \\ |x_2| & \text{if } |x_2| < |x_1| \end{cases}$$

and

$$r_> = \begin{cases} |x_2| & \text{if } |x_1| < |x_2| \\ |x_1| & \text{if } |x_2| < |x_1| \end{cases} .$$

This form leads to the multipole expansion of the Coulomb-gauge (or static) electric potential

$$\phi(\vec{x}, t) = \int \frac{\rho(y,t)\, d^3y}{|\vec{x} - \vec{y}|}$$

$$= \sum_{\ell=0}^{\infty} \frac{1}{2\ell+1} \sum_{m=-\ell}^{\ell} \frac{Y_\ell^m(\theta_x, \phi_x)}{|x|^{\ell+1}} \int d^3y \, Y_\ell^{m*}(\theta_y, \phi_y) |y|^\ell \rho(\vec{y}, t)$$

in which the charge density $\rho(\vec{y}, t)$ is taken to vanish for $|y| > r$ and in which $|\vec{x}| > r$.

One has (12.4a)

$$\frac{1}{|\vec{r}_1 - \vec{r}_2|} = \sum_{\ell=0}^{\infty} \frac{r_<^{\ell}}{r_>^{\ell+1}} P_\ell\left(\frac{\vec{r}_1 \cdot \vec{r}_2}{r_1 r_2}\right).$$

and also

$$P_\ell(\hat{r}_1 \cdot \hat{r}_2) = \frac{4\pi}{2\ell+1} \sum_{m=-\ell}^{\ell} Y_\ell^m(\theta_1, \phi_1) Y_\ell^{m*}(\theta_2, \phi_2),$$

A differential operator of the form

$$\mathcal{L} = \frac{d}{dx}\left(p(x) \frac{d}{dx} \right) + q(x)$$

is said to be in <u>self-adjoint form.</u>

Why is that good? If $\mathcal{L}$ is self adjoint, then

$$\mathcal{L} u = (p u')' + q u$$

and

$$\int_a^b v^* \mathcal{L} u \, dx = \int_a^b v^* \left[(p u')' + q u \right] dx$$

$$= \int_a^b \left[-p u' v^{*\prime} + u q v^* \right] dx + \left[v^* p u' \right]_a^b$$

$$= \int_a^b \left[u p v^{*\prime\prime} + u q v^* \right] dx - \left[p u v^{*\prime} \right]_a^b + \left[v^* p u' \right]_a^b$$

$$= \int_a^b u \mathcal{L} v^* dx + \left[v^* p u' - v^{*\prime} p u \right]_a^b$$

Suppose now that the boundary terms vanish. Then

$$\int_a^b v^* \mathcal{L} u \, dx = \int_a^b u \mathcal{L} v^* dx = \int_a^b (\mathcal{L} v^*) u \, dx.$$

If in fact p and q are real so that $\mathcal{L}^* = \mathcal{L}$, then

$$\int_a^b v^* \mathcal{L} u \, dx = \int_a^b (\mathcal{L} v)^* u \, dx = \left(\int_a^b u^* \mathcal{L} v \, dx \right)^*$$

$$\int_a^b v^* \mathcal{L}^\dagger u \, dx$$

$$\langle v | \mathcal{L} | u \rangle = \langle v | \mathcal{L}^\dagger | u \rangle = \langle u | \mathcal{L} | v \rangle^*$$

which we interpret as $\mathcal{L} = \mathcal{L}^\dagger$, ie, the operator $\mathcal{L}$ is hermitian. So a self-adjoint $\mathcal{L}$ with real p & q is hermitian.

The self-adjoint character of $\mathcal{L}$ is effective only if

$\left[p(v^* u' - v^{*\prime} u) \right]_a^b = 0$. So one must choose a and b carefully to fit each problem. Usually, people require that all the functions u and v to which $\mathcal{L}$ is applied satisfy the boundary conditions

$$p v^* u' \Big]_a^b = 0 = p u v^{*\prime} \Big]_a^b .$$

Sometimes, one even insists that

$$p v^* u' \Big|_{x=a} = 0 = p v^* u' \Big|_{x=b}$$

$$p u^* v' \Big|_{x=a} = 0 \quad p u^* v' \Big|_{x=b}$$

but these extra conditions are not necessary.

In some cases a and b are taken to be $a = -\infty$ and $b = +\infty$, and it is assumed that

$$0 = p v^* u' \quad \text{etc at} \quad x = \pm\infty.$$

One might imagine that self-adjoint operators are rare. But in fact one can multiply the generic 2d-order differential operator

$$\mathcal{L}_0 u = p_0 u'' + p_1 u' + p_2 u$$

by
$$\frac{1}{p_0} e^{\int^x \frac{p_1(t)}{p_0(t)} dt}$$

and get a self-adjoint $\mathcal{L}$:

$$\frac{1}{p_0} e^{\int^x \frac{p_1}{p_0} dt} \mathcal{L}_0 u = e^{\int^x p_1/p_0 dt} u'' + \frac{p_1}{p_0} e^{\int^x p_1/p_0 dt} u'$$

$$+ \frac{p_2}{p_0} e^{\int^x p_1/p_0 dt} u$$

$$= \left\{ \exp\left[\int^x \frac{p_1(t) dt}{p_0(t)}\right] u' \right\}' + \frac{p_2}{p_0} \exp \int \frac{p_1}{p_0} dt \; u$$

$$= (p u')' + q u \quad \text{where}$$

$$p = \exp\left[\int^x \frac{p_1(t)}{p_0(t)} dt\right] \quad \text{and} \quad q = \frac{p_2}{p_0} p.$$

So we always may cast a 2d-order differential operator into self-adjoint form, $\mathcal{L}$. And if p & q are real, then $\mathcal{L}$ is hermitian on functions u and v that satisfy the boundary conditions

$$\left[p \left(v^* u' - v^{*\prime} u \right) \right]_a^b = 0 .$$

Eigen This and That

Suppose

$$\lambda w u + \mathcal{L} u = (p u')' + q u + \lambda w u = 0 \qquad \text{ie}$$

$$(p(x)\, u'(x))' + q(x)\, u(x) + \lambda\, w(x)\, u(x) = 0,$$

then λ is said to be the Eigen<u>value</u> and $w(x)$ is a known weight or density function. Here $w(x) \geq 0$ and $w(x) = 0$ only at isolated points. '<u>Eigen</u>' means 'special' in Deutsch.

Legendre's eq. is a good example. It is

$$0 = \mathcal{L} y = (1-x^2) y'' - 2 x y' + \ell(\ell+1) y$$

$$0 = ((1-x^2) y')' + \ell(\ell+1) y$$

As you will show when you do HW problem 8.5.5, series solutions exist for each of the two solutions $k=0$ and $k=1$ of the indicial equation

$$k(k-1)=0,$$

but the resulting series diverge for $x=\pm 1$ (i.e., $\theta = 0$ or π) unless l is an integer. This is why orbital angular momentum is quantized. So the eigenvalue is $l(l+1)$ for integral l.

The deuteron is a spin-1 bound state of a neutron and a proton with binding energy about 2.2 MeV. It is mostly an S-state with some d-state mixed in. So the spins of the n and p are aligned. If r is the relative distance in the reduced-mass formalism, then

$$-\frac{\hbar^2}{2m}\Delta\psi + V\psi = E\psi, \qquad V(r) = \begin{cases} V_0 < 0 & \text{if } r<a \\ 0 & \text{if } r>a \end{cases}$$

For an s-state boils down to this equation

$$u'' + k_1^2 u = 0 \qquad\qquad u'' - k_2^2 u = 0$$

for $u(r) = r\psi(r)$ where $k_1^2 = \frac{2M}{\hbar^2}(E - V_0) > 0$ for $0 \le r \le a$ and

$$k_2^2 = -\frac{2ME}{\hbar^2} > 0$$

for $a \le r$.

So $u(r) = \alpha \sin k_1 r + \beta \cos k_1 r$ for $r < a$, but $\beta = 0$ to avoid a singularity at $r = 0$ in

$$\psi(r) = \frac{u(r)}{r}.$$

Outside the square well,

$$u = A e^{k_2 r} + B e^{-k_2 r},$$

but $A = 0$ so that ψ can be normalized.

When one matches the two solutions at the boundary, $r = a$, by requiring that

$$u_1(a) = \alpha \sin k_1 a = B e^{-k_2 a} = u_2(a) \quad \text{and}$$

$$u_1'(a) = \alpha k_1 \cos k_1 a = -k_2 B e^{-k_2 a} = u_2'(a),$$

one finds that

$$\tan k_1 a = -\frac{k_1}{k_2} = -\sqrt{\frac{E - V_0}{-E}}, \quad E < 0, \; V_0 < 0.$$

i.e.,

$$\tan\left(\sqrt{\frac{2Ma^2}{\hbar^2}(E - V_0)}\right) = -\sqrt{\frac{E - V_0}{-E}}$$

which has only discrete, quantized solutions for $E < 0$ and $V_0 < 0$, $|V_0| > |E|$.

$\mathcal{L}$ is 2d order. What about first-order Hermitian operators? Some examples are

$$\vec{p} = \frac{\hbar}{i}\vec{\nabla} \quad \text{or in one dimension} \quad p = \frac{\hbar}{i}\frac{d}{dx}.$$

In this case

$$\int_a^b dx\, v^* p u = \int_a^b dx\, v^* \frac{\hbar}{i} u' = -\int_a^b dx\, u \frac{\hbar}{i} v^{*\prime} + \frac{\hbar}{i}\left[v^* u\right]_a^b$$

$$= \int_a^b dx\, u \left(\frac{\hbar}{i} v'\right)^* + \frac{\hbar}{i}\left[v^* u\right]_a^b$$

So if

$$0 = \left[v^* u\right]_a^b = v^*(b)\, u(b) - v^*(a)\, u(a),$$

then

$$\int_a^b dx\, v^* p u = \left(\int_a^b dx\, u^* p v\right)^* = \int_a^b dx\, (p^\dagger v)^* u$$

$$= \int_a^b dx\, (p v)^* u \qquad \text{so} \quad p = p^\dagger.$$

The trick is in the i, and in the boundary conditions

$$0 = \left[v^* u\right]_a^b$$

which often are satisfied when $a \to -\infty$, $b \to +\infty$, and both u and v are normalized.