Verifying the Helmholtz Green's function.

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Peeter Joot — peeter.joot@gmail.com

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1. Motivation.

In class this week, looking at an instance of the Helmholtz equation

$$\left(\boldsymbol{\nabla}^2 + \mathbf{k}^2\right)\psi_{\mathbf{k}}(\mathbf{r}) = s(\mathbf{r}).$$
(1)

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We were told that the Green's function

$$\left(\boldsymbol{\nabla}^2 + \mathbf{k}^2\right) G^0(\mathbf{r}, \mathbf{r}') = \delta(\mathbf{r} - \mathbf{r}')$$
(2)

that can be used to solve for a particular solution this differential equation via convolution

$$\psi_{\mathbf{k}}(\mathbf{r}) = \int G^0(\mathbf{r}, \mathbf{r}') s(\mathbf{r}') d^3 \mathbf{r}', \qquad (3)$$

had the value

$$G^{0}(\mathbf{r},\mathbf{r}') = -\frac{1}{4\pi} \frac{e^{ik|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r}-\mathbf{r}'|}.$$
(4)

Let's try to verify this.

2. Guts

Application of the Helmholtz differential operator $\nabla^2 + \mathbf{k}^2$ on the presumed solution gives

$$(\boldsymbol{\nabla}^2 + \mathbf{k}^2)\psi_{\mathbf{k}}(\mathbf{r}) = -\frac{1}{4\pi} \int (\boldsymbol{\nabla}^2 + \mathbf{k}^2) \frac{e^{ik|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r}-\mathbf{r}'|} s(\mathbf{r}') d^3\mathbf{r}'.$$
(5)

2.1. When $\mathbf{r} \neq \mathbf{r}'$.

To proceed we'll need to evaluate

$$\nabla^2 \frac{e^{ik|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r}-\mathbf{r}'|}.$$
(6)

Writing $\mu = |\mathbf{r} - \mathbf{r}'|$ we start with the computation of

$$\frac{\partial}{\partial x}\frac{e^{ik\mu}}{\mu} = \frac{\partial\mu}{\partial x}\left(\frac{ik}{\mu} - \frac{1}{\mu^2}\right)e^{ik\mu}$$
$$= \frac{\partial\mu}{\partial x}\left(ik - \frac{1}{\mu}\right)\frac{e^{ik\mu}}{\mu}$$

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We see that we'll have

$$\boldsymbol{\nabla}\frac{e^{ik\mu}}{\mu} = \left(ik - \frac{1}{\mu}\right)\frac{e^{ik\mu}}{\mu}\boldsymbol{\nabla}\mu.$$
(7)

Taking second derivatives with respect to *x* we find

$$\frac{\partial^2}{\partial x^2} \frac{e^{ik\mu}}{\mu} = \frac{\partial^2 \mu}{\partial x^2} \left(ik - \frac{1}{\mu} \right) \frac{e^{ik\mu}}{\mu} + \frac{\partial \mu}{\partial x} \frac{\partial \mu}{\partial x} \frac{1}{\mu^2} \frac{e^{ik\mu}}{\mu} + \left(\frac{\partial \mu}{\partial x} \right)^2 \left(ik - \frac{1}{\mu} \right)^2 \frac{e^{ik\mu}}{\mu} \\ = \frac{\partial^2 \mu}{\partial x^2} \left(ik - \frac{1}{\mu} \right) \frac{e^{ik\mu}}{\mu} + \left(\frac{\partial \mu}{\partial x} \right)^2 \left(-k^2 - \frac{2ik}{\mu} + \frac{2}{\mu^2} \right) \frac{e^{ik\mu}}{\mu}.$$

Our Laplacian is then

$$\boldsymbol{\nabla}^2 \frac{e^{ik\mu}}{\mu} = \left(ik - \frac{1}{\mu}\right) \frac{e^{ik\mu}}{\mu} \boldsymbol{\nabla}^2 \mu + \left(-k^2 - \frac{2ik}{\mu} + \frac{2}{\mu^2}\right) \frac{e^{ik\mu}}{\mu} (\boldsymbol{\nabla}\mu)^2. \tag{8}$$

Now lets calculate the derivatives of μ . Working on *x* again, we have

$$\begin{split} \frac{\partial}{\partial x}\mu &= \frac{\partial}{\partial x}\sqrt{(x-x')^2 + (y-y')^2 + (z-z')^2} \\ &= \frac{1}{2}2(x-x')\frac{1}{\sqrt{(x-x')^2 + (y-y')^2 + (z-z')^2}} \\ &= \frac{x-x'}{\mu}. \end{split}$$

So we have

$$\boldsymbol{\nabla}\boldsymbol{\mu} = \frac{\mathbf{r} - \mathbf{r}'}{\boldsymbol{\mu}} \tag{9}$$

$$(\boldsymbol{\nabla}\boldsymbol{\mu})^2 = 1 \tag{10}$$

Taking second derivatives with respect to x we find

$$\begin{aligned} \frac{\partial^2}{\partial x^2} \mu &= \frac{\partial}{\partial x} \frac{x - x'}{\mu} \\ &= \frac{1}{\mu} - (x - x') \frac{\partial \mu}{\partial x} \frac{1}{\mu^2} \\ &= \frac{1}{\mu} - (x - x') \frac{x - x'}{\mu} \frac{1}{\mu^2} \\ &= \frac{1}{\mu} - (x - x')^2 \frac{1}{\mu^3}. \end{aligned}$$

So we find

$$\boldsymbol{\nabla}^2 \boldsymbol{\mu} = \frac{3}{\boldsymbol{\mu}} - \frac{1}{\boldsymbol{\mu}},\tag{11}$$

or

$$\boldsymbol{\nabla}^2 \boldsymbol{\mu} = \frac{2}{\boldsymbol{\mu}}.$$

Inserting this and $(\nabla \mu)^2$ into 8 we find

$$\boldsymbol{\nabla}^2 \frac{e^{ik\mu}}{\mu} = \left(ik - \frac{1}{\mu}\right) \frac{e^{ik\mu}}{\mu} \frac{2}{\mu} + \left(-k^2 - \frac{2ik}{\mu} + \frac{2}{\mu^2}\right) \frac{e^{ik\mu}}{\mu} = -k^2 \frac{e^{ik\mu}}{\mu}$$
(13)

This shows us that provided $\mathbf{r} \neq \mathbf{r}'$ we have

$$(\boldsymbol{\nabla}^2 + \mathbf{k}^2)G^0(\mathbf{r}, \mathbf{r}') = 0.$$
(14)

2.2. In the neighborhood of $|\mathbf{r} - \mathbf{r}'| < \epsilon$.

Having shown that we end up with zero everywhere that $\mathbf{r} \neq \mathbf{r}'$ we are left to consider a neighborhood of the volume surrounding the point \mathbf{r} in our integral. Following the Coulomb treatment in §2.2 of [1] we use a spherical volume element centered around \mathbf{r} of radius ϵ , and then convert a divergence to a surface area to evaluate the integral away from the problematic point

$$-\frac{1}{4\pi} \int_{\text{all space}} (\nabla^2 + \mathbf{k}^2) \frac{e^{ik|\mathbf{r} - \mathbf{r}'|}}{|\mathbf{r} - \mathbf{r}'|} s(\mathbf{r}') d^3 \mathbf{r}' = -\frac{1}{4\pi} \int_{|\mathbf{r} - \mathbf{r}'| < \epsilon} (\nabla^2 + \mathbf{k}^2) \frac{e^{ik|\mathbf{r} - \mathbf{r}'|}}{|\mathbf{r} - \mathbf{r}'|} s(\mathbf{r}') d^3 \mathbf{r}'$$
(15)

We make the change of variables $\mathbf{r}' = \mathbf{r} + \mathbf{a}$. We add an explicit \mathbf{r} suffix to our Laplacian at the same time to remind us that it is taking derivatives with respect to the coordinates of $\mathbf{r} = (x, y, z)$, and not the coordinates of our integration variable $\mathbf{a} = (a_x, a_y, a_z)$. Assuming sufficient continuity and "well behavedness" of $s(\mathbf{r}')$ we'll be able to pull it out of the integral, giving

$$\begin{aligned} -\frac{1}{4\pi} \int_{|\mathbf{r}-\mathbf{r}'|<\epsilon} (\mathbf{\nabla}_{\mathbf{r}}^2 + \mathbf{k}^2) \frac{e^{ik|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r}-\mathbf{r}'|} s(\mathbf{r}') d^3 \mathbf{r}' &= -\frac{1}{4\pi} \int_{|\mathbf{a}|<\epsilon} (\mathbf{\nabla}_{\mathbf{r}}^2 + \mathbf{k}^2) \frac{e^{ik|\mathbf{a}|}}{|\mathbf{a}|} s(\mathbf{r}+\mathbf{a}) d^3 \mathbf{a} \\ &= -\frac{s(\mathbf{r})}{4\pi} \int_{|\mathbf{a}|<\epsilon} (\mathbf{\nabla}_{\mathbf{r}}^2 + \mathbf{k}^2) \frac{e^{ik|\mathbf{a}|}}{|\mathbf{a}|} d^3 \mathbf{a} \end{aligned}$$

Recalling the dependencies on the derivatives of $|\mathbf{r}-\mathbf{r}'|$ in our previous gradient evaluations, we note that we have

$$\nabla_{\mathbf{r}} |\mathbf{r} - \mathbf{r}'| = -\nabla_{\mathbf{a}} |\mathbf{a}| \tag{16}$$

$$(\boldsymbol{\nabla}_{\mathbf{r}} |\mathbf{r} - \mathbf{r}'|)^2 = (\boldsymbol{\nabla}_{\mathbf{a}} |\mathbf{a}|)^2$$
(17)

$$\boldsymbol{\nabla}_{\mathbf{r}}^{2} |\mathbf{r} - \mathbf{r}'| = \boldsymbol{\nabla}_{\mathbf{a}}^{2} |\mathbf{a}|, \qquad (18)$$

so with $\mathbf{a} = \mathbf{r} - \mathbf{r}'$, we can rewrite our Laplacian as

$$\boldsymbol{\nabla}_{\mathbf{r}}^{2} \frac{e^{ik|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r}-\mathbf{r}'|} = \boldsymbol{\nabla}_{\mathbf{a}}^{2} \frac{e^{ik|\mathbf{a}|}}{|\mathbf{a}|} = \boldsymbol{\nabla}_{\mathbf{a}} \cdot \left(\boldsymbol{\nabla}_{\mathbf{a}} \frac{e^{ik|\mathbf{a}|}}{|\mathbf{a}|}\right)$$
(19)

This gives us

$$\begin{aligned} -\frac{s(\mathbf{r})}{4\pi} \int_{|\mathbf{a}|<\epsilon} (\nabla_{\mathbf{a}}^{2} + \mathbf{k}^{2}) \frac{e^{ik|\mathbf{a}|}}{|\mathbf{a}|} d^{3}\mathbf{a} &= -\frac{s(\mathbf{r})}{4\pi} \int_{dV} \nabla_{\mathbf{a}} \cdot \left(\nabla_{\mathbf{a}} \frac{e^{ik|\mathbf{a}|}}{|\mathbf{a}|} \right) d^{3}\mathbf{a} - \frac{s(\mathbf{r})}{4\pi} \int_{dV} \mathbf{k}^{2} \frac{e^{ik|\mathbf{a}|}}{|\mathbf{a}|} d^{3}\mathbf{a} \\ &= -\frac{s(\mathbf{r})}{4\pi} \int_{dA} \left(\nabla_{\mathbf{a}} \frac{e^{ik|\mathbf{a}|}}{|\mathbf{a}|} \right) \cdot \hat{\mathbf{a}} d^{2}\mathbf{a} - \frac{s(\mathbf{r})}{4\pi} \int_{dV} \mathbf{k}^{2} \frac{e^{ik|\mathbf{a}|}}{|\mathbf{a}|} d^{3}\mathbf{a} \end{aligned}$$

To complete these evaluations, we can now employ a spherical coordinate change of variables. Let's do the k^2 volume integral first. We have

$$\begin{split} \int_{dV} \mathbf{k}^2 \frac{e^{ik|\mathbf{a}|}}{|\mathbf{a}|} d^3 \mathbf{a} &= \int_{a=0}^{\epsilon} \int_{\theta=0}^{\pi} \int_{\phi=0}^{2\pi} \mathbf{k}^2 \frac{e^{ika}}{a} a^2 da \sin \theta d\theta d\phi \\ &= 4\pi k^2 \int_{a=0}^{\epsilon} a e^{ika} da \\ &= 4\pi \int_{u=0}^{k\epsilon} u e^{iu} du \\ &= 4\pi \left(-iu + 1 \right) e^{iu} \Big|_{0}^{k\epsilon} \\ &= 4\pi \left((-ik\epsilon + 1) e^{ik\epsilon} - 1 \right) \end{split}$$

To evaluate the surface integral we note that we'll require only the radial portion of the gradient, so have

$$\left(\boldsymbol{\nabla}_{\mathbf{a}} \frac{e^{ik|\mathbf{a}|}}{|\mathbf{a}|}\right) \cdot \hat{\mathbf{a}} = \left(\hat{\mathbf{a}} \frac{\partial}{\partial a} \frac{e^{ika}}{a}\right) \cdot \hat{\mathbf{a}}$$
$$= \frac{\partial}{\partial a} \frac{e^{ika}}{a}$$
$$= \left(ik\frac{1}{a} - \frac{1}{a^2}\right) e^{ika}$$
$$= (ika - 1) \frac{e^{ika}}{a^2}$$

Our area element is $a^2 \sin \theta d\theta d\phi$, so we are left with

$$\int_{dA} \left(\nabla_{\mathbf{a}} \frac{e^{ik|\mathbf{a}|}}{|\mathbf{a}|} \right) \cdot \hat{\mathbf{a}} d^{2}\mathbf{a} = \int_{\theta=0}^{\pi} \int_{\phi=0}^{2\pi} (ika-1) \frac{e^{ika}}{a^{2}} a^{2} \sin\theta d\theta d\phi \Big|_{a=\epsilon}$$

$$= 4\pi (ik\epsilon - 1) e^{ik\epsilon}$$
(20)

Putting everything back together we have

$$-\frac{1}{4\pi} \int_{\text{all space}} (\boldsymbol{\nabla}^2 + \mathbf{k}^2) \frac{e^{ik|\mathbf{r} - \mathbf{r}'|}}{|\mathbf{r} - \mathbf{r}'|} s(\mathbf{r}') d^3 \mathbf{r}' = -s(\mathbf{r}) \left((-ik\epsilon + 1)e^{ik\epsilon} - 1 + (ik\epsilon - 1)e^{ik\epsilon} \right)$$
$$= -s(\mathbf{r}) \left((-ik\epsilon + 1 + ik\epsilon - 1)e^{ik\epsilon} - 1 \right)$$

But this is just

$$-\frac{1}{4\pi}\int_{\text{all space}} (\boldsymbol{\nabla}^2 + \mathbf{k}^2) \frac{e^{ik|\mathbf{r} - \mathbf{r}'|}}{|\mathbf{r} - \mathbf{r}'|} s(\mathbf{r}') d^3 \mathbf{r}' = s(\mathbf{r}).$$
(21)

This completes the desired verification of the Green's function for the Helmholtz operator. Observe the perfect cancellation here, so the limit of $\epsilon \rightarrow 0$ can be independent of how large k is made. You have to complete the integrals for both the Laplacian and the \mathbf{k}^2 portions of the integrals and add them, <u>before</u> taking any limits, or else you'll get into trouble (as I did in my first attempt).

References

[1] M. Schwartz. Principles of Electrodynamics. Dover Publications, 1987. 2.2