Green's Function in Free Space

Example: Solve $\nabla^2 G(\mathbf{r},\mathbf{r}') = -\delta(\mathbf{r}-\mathbf{r}')$ using the Fourier's transformation.

Answer:

Start with the Fourier transformation in one dimension:

$$f(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{ikx} f(k)dk_x \quad \Rightarrow \quad \nabla^2 f(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty} (-ik)^2 e^{ikx} f(k)dk_x$$

In three dimensions:

$$f(\mathbf{r}) = \frac{1}{(2\pi)^3}\int_{-\infty}^{\infty} e^{i\,\mathbf{k}\cdot\mathbf{r}} f(\mathbf{k})d\,\mathbf{k} \quad \Rightarrow \quad \nabla^2 f(\mathbf{r}) = \frac{1}{(2\pi)^3}\int_{-\infty}^{\infty} (-ik)^2 e^{i\,\mathbf{k}\cdot\mathbf{r}} f(\mathbf{k})d\,\mathbf{k}$$

For a continuous function in three dimensions, one finds:

$$\delta(\mathbf{r}-\mathbf{r'}) = \frac{1}{(2\pi)^3}\int_{-\infty}^{\infty} e^{i\,\vec{\mathrm{k}}.(\mathbf{r}-\mathbf{r}')} d^3k$$

Thus $\nabla^2 G(\mathbf{r},\mathbf{r}') = -\delta(\mathbf{r}-\mathbf{r}')$ will be (change G with F:

$$\nabla^2 f(\mathbf{r}) + \delta(\mathbf{r}-\mathbf{r}') = \frac{1}{(2\pi)^3}\int_{-\infty}^{\infty} (-ik)^2 e^{i\,\mathbf{k}\cdot\mathbf{r}} f(\mathbf{k})d\,\mathbf{k} + \frac{1}{(2\pi)^3}\int_{-\infty}^{\infty} e^{i\,\vec{\mathrm{k}}.(\mathbf{r}-\mathbf{r}')} d^3k = 0$$

This implies:

$$\frac{1}{(2\pi)^3}\int_{-\infty}^{\infty} \left\{(-k^2) f(\mathbf{k}) + e^{-i\,\mathbf{k}\cdot\mathbf{r}'}\right\} e^{i\,\mathbf{k}\cdot\mathbf{r}} d^3k = 0$$

Consequently,

$$\Rightarrow \quad -k^2 f(\mathbf{k}) + e^{-i\,\mathbf{k}\cdot\mathbf{r}'} = 0 \quad \Rightarrow \quad \boxed{f(\mathbf{k}) = \frac{e^{-i\,\mathbf{k}\cdot\mathbf{r}'}}{k^2}}$$

Thus:

$$G(\mathbf{r}-\mathbf{r'}) = \frac{1}{(2\pi)^3}\int e^{i\,\mathbf{k}\cdot\mathbf{r}} f(\mathbf{k})d\,\mathbf{k} = \frac{1}{(2\pi)^3}\int e^{i\,\mathbf{k}.\mathbf{r}} \frac{e^{-i\,\mathbf{k}\cdot\mathbf{r}'}}{k^2} d\,\mathbf{k}$$

$$= \frac{1}{(2\pi)^3}\int \frac{e^{i\,\mathbf{k}\cdot\mathbf{R}}}{k^2} d\,\mathbf{k}^*, \qquad \mathbf{R = r - r'}$$

H.W. Do the integration with the notations:

$d\,\mathbf{k} = k^2 dk d\Omega = k^2 dk \sin\theta d\theta d\phi$ and $\mathbf{k}\cdot\mathbf{R} = kr\cos\theta$, one finds:

Answer:

$$G(\mathbf{r}-\mathbf{r'}) = \frac{1}{2\pi^2 R}\underbrace{\int_0^{\infty}\frac{\sin(kr)}{k}dk}_{\pi/2} = \frac{1}{4\pi R} = \frac{1}{4\pi|\mathbf{r - r'}|}$$

[*Help: prove the standard integral $I_1 = \int \frac{e^{-br\pm i\,\boldsymbol{q}\cdot\mathbf{r}}}{r} d\tau = \frac{4\pi}{b^2+q^2}$]

Prove that the Green's function $G(\mathbf{r}) = \frac{e^{\pm ikr}}{r}$ is the solution of the scalar wave equation:

$$\left(\nabla^2 \pm k^2\right) G(\mathbf{r}) = -4\pi\delta(\mathbf{r}) \tag{1}$$

Proof: We have two cases:

Case I: $r \neq 0$, we have to prove that $\left(\nabla^2 + k^2\right)\left(\frac{e^{ikr}}{r}\right) = 0$

Start with $\nabla^2\left(\frac{e^{ikr}}{r}\right) = \frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{d}{dr}(\frac{e^{ikr}}{r})\right) = -\frac{k^2}{r}e^{ikr}$, $\Rightarrow$ $\left(\nabla^2 + k^2\right)\left(\frac{e^{ikr}}{r}\right) = 0,$

Case II: $r = 0$, we have to prove that $\int\left(\nabla^2 + k^2\right)G(\mathbf{r})d^3r = -4\pi\int\delta(\mathbf{r})d^3r = -4\pi$

In this case let us construct the solution of a scalar wave equation in any volume V of free space having an arbitrary small radius ξ and having an arbitrary source $\rho(\mathbf{r})$, then

a)

$$\int\limits_{\text{sphere of radius } \xi} \nabla^2 G(\mathbf{r})d^3r = \int\nabla\cdot\left(\nabla G(\mathbf{r})\right)d^3r \underbrace{=}_{\text{using the Green's identity}} \int\nabla G(\mathbf{r})\cdot d\vec{\text{s}}$$

$$= \int\hat{\text{r}}\frac{d}{dr}\left(\frac{e^{ikr}}{r}\right)\cdot\hat{\text{r}}\, r^2 d\Omega \tag{A}$$

$$= 4\pi\left[ik\,\xi e^{ik\xi} - e^{ik\xi}\right]$$

b)

$$k^2\int G(\mathbf{r})d^3r = k^2\int\frac{e^{ikr}}{r}r^2\,drd\Omega$$

$$= 4\pi\left[\left(\frac{e^{ikr}}{ik}\right)\Bigg|_0^{\xi} - \frac{1}{ik}\int_0^{\xi}e^{ikr}dr\right] \tag{B}$$

$$= 4\pi\left[-ik\,\xi e^{ik\xi} + e^{ik\xi} - 1\right]$$

From the final results of equations A and B, one finds

$$\int\left(\nabla^2 + k^2\right)G(\mathbf{r})d^3r = -4\pi$$

Fourier transformation

Example: Find the Fourier transformation of the function $f\ (r)=\dfrac{e^{-r}}{r}$.{Hint: use the spherical coordinates where $d\tau = r^2 \sin\theta d\theta d\varphi dr$]

. **Solution:** $f\ (\mathbf{r})=\dfrac{e^{-r}}{r} \Rightarrow \quad f\ (\mathbf{q})=\dfrac{1}{(2\pi)^{3/2}}\int \dfrac{e^{-r+i\ \mathbf{q}\cdot\mathbf{r}}}{r} d\tau, \qquad d\tau = r^2 \sin\theta d\theta d\varphi dr$

$$I_1=\int \frac{e^{-br+i\,\boldsymbol{q}\cdot\boldsymbol{r}}}{r} d\boldsymbol{r} = \int_0^{2\pi} d\phi \int_0^{\infty} r^2 dr \left[\int_{-1}^{1} d\cos\theta e^{iqr\cos\theta}\right]\frac{e^{-br}}{r}$$

$$=2\pi\int_0^{\infty} r^2 dr\left[\frac{e^{iqr}-e^{-iqr}}{iqr}\right]\frac{e^{-br}}{r} = \frac{2\pi}{iq}\int_0^{\infty} dr\left[e^{(iq-b)r}-e^{-(iq+b)r}\right]$$

$$=\frac{2\pi}{iq}\left[\frac{e^{(iq-b)r}\Big|_0^{\infty}}{iq-b}+\frac{e^{-(iq+b)r}\Big|_0^{\infty}}{iq+b}\right] = -\frac{2\pi}{iq}\left[\frac{1}{iq-b}+\frac{1}{iq+b}\right]=\frac{4\pi}{b^2+q^2}$$

$$\therefore f\ (\mathbf{q})=\frac{1}{(2\pi)^{3/2}}\int \frac{e^{-r+i\ \mathbf{q}\cdot\mathbf{r}}}{r} d\tau = \frac{1}{(2\pi)^{3/2}}\frac{4\pi}{1+q^2}=\sqrt{\frac{2}{\pi}}\frac{1}{1+q^2}$$

Example: Find the Fourier transformation of the function $f\ (\mathbf{r})=e^{-br}$. [Hint:

$I_1=\int \dfrac{e^{-br\pm i\,\boldsymbol{q}\cdot\boldsymbol{r}}}{r} d\tau = \dfrac{4\pi}{b^2+q^2}$] ,

$$f\ (\mathbf{r})=e^{-r} \Rightarrow f\ (\mathbf{q})=\frac{1}{(2\pi)^{3/2}}\int e^{-br+i\ \mathbf{q}\cdot\mathbf{r}} d\tau$$

$$=\frac{1}{(2\pi)^{3/2}}\frac{-\partial}{\partial b}\left[\int \frac{e^{-br\pm i\,\boldsymbol{q}\cdot\boldsymbol{r}}}{r} d\tau\right]=\frac{1}{(2\pi)^{3/2}}\frac{-\partial}{\partial b}\frac{4\pi}{b^2+q^2}=\frac{1}{(2\pi)^{3/2}}\frac{8\pi b}{(b^2+q^2)^2}$$

H.W. Calculate the following integrals:

$$I=\int \frac{e^{i\,\boldsymbol{k}\cdot\boldsymbol{R}}}{k^2} d\boldsymbol{k} = \frac{2\pi^2}{R}$$

$$I_2=\int e^{-br\pm i\,\boldsymbol{q}\cdot\boldsymbol{r}} d\tau = -\frac{\partial I_1}{\partial b}=\frac{8\pi b}{(b^2+q^2)^2};$$

$$I_3=\int \frac{e^{\pm i\,\boldsymbol{q}\cdot\boldsymbol{r}}}{|\mathrm{r}-\mathrm{r}'|} d\boldsymbol{r} = e^{\pm i\boldsymbol{q}\cdot\boldsymbol{r}'}\int \frac{e^{\pm i\,\boldsymbol{q}\cdot(\mathrm{r}-\mathrm{r}')}}{|\mathrm{r}-\mathrm{r}'|} d\boldsymbol{r} = e^{\pm i\boldsymbol{q}\cdot\boldsymbol{r}'}\lim_{b\to 0} I_1 = \frac{4\pi}{q^2}e^{\pm i\boldsymbol{q}\cdot\boldsymbol{r}'}$$

Example: Calculate the Fourier transformation of the Gaussian function $f\ (x)=e^{-x^2}$.

Answer:

$$g(k)=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} e^{-x^2-ikx} dx = \frac{e^{-k^2/4}}{\sqrt{2\pi}}\underbrace{\int_{-\infty}^{\infty} e^{-\left(x^2+\frac{ik}{2}\right)^2} dx}_{\sqrt{\pi}} = \frac{e^{-k^2/4}}{\sqrt{2}}$$

Note that: The Fourier transform of a Gaussian functions is a Gaussian function.

Prove that if $f(x) = Ne^{-\alpha x^2}$, then $g(k) = \frac{N}{\sqrt{2\alpha}} e^{-k^2/(4\alpha)}$, and vice versa.

Integrals in *D* dimensions

In polar coordinates the *D*-dimensional volume element reads:

$$d^D x = r^{D-1} dr \sin^{D-2}\theta_{D-1} d\theta_{D-1} \sin^{D-3}\theta_{D-2} d\theta_{D-2} \cdots \left(d\theta_1 = d\varphi\right)$$

$0 \le \theta_1 \le 2\pi, \quad 0 \le \theta_k \le 2\pi, \quad k \ne 1$

Very often the integrand is independent of the angles; then one needs only the surface area of the *D*-dimensional sphere:

$$d^D x = S_D r^{D-1} dr$$

This is easily found by evaluating in two different ways the integral

$$J = \int d^D x \; e^{-(x_1^2 + x_2^2 + \cdots + x_D^2)} = \left[\int dx\, e^{-x^2}\right]^D = \pi^{D/2}$$

$$J = S_D \int_0^\infty r^{D-1} e^{-r^2} dr = \frac{1}{2} S_D \Gamma\left(\frac{D}{2}\right)$$

Whence

$$S_D = \frac{2\pi^{D/2}}{\Gamma(D/2)}$$

Examples:

D	S_D
1	2
2	2π
3	4π
4	$2\pi^2$

The volume is given by:

$$V = \int_0^R S_D R^{D-1} dR = \frac{\pi^{D/2}}{\Gamma\left(\frac{D}{2}+1\right)} R^D$$

Examples:

D	V
1	2 R
2	πR^2
3	$\frac{4\pi R^3}{3}$
4	$\frac{\pi^2 R^4}{2}$

As a rule, the integration measure is $d^D x / (2\pi)^D$, and it proves useful to define:

$$K_D = \frac{S_D}{(2\pi)^D} = \frac{2}{(4\pi)^{D/2}\Gamma(D/2)}.$$ In particular $K_4 = \frac{1}{8\pi^2}$

Volume of a Hypersphere

Consider the integral

$$I = \int_{-\infty}^{\infty} \exp[-(x_1^2 + x_2^2 + \cdots + x_n^2)] dx_1\, dx_2 \cdots dx_n$$
$$= \left[\int_{-\infty}^{\infty} \exp(-x^2) dx\right]^n = \pi^{n/2}. \qquad (1)$$

For the n-dimensional sphere of volume V_n, the surface area can be written as $r^{n-1} S_n$. Therefore, we also have

$$I = \int_0^{\infty} \exp(-r^2) r^{n-1} S_n\, dr$$
$$= \frac{1}{2} S_n \int_0^{\infty} \exp(-t) t^{(n-2)/2} dt = \frac{1}{2} S_n \Gamma\left(\frac{n}{2}\right), \qquad (2)$$

where we have used (4).

From (1) and (2)

$$* \int_0^{\infty} t^n e^{-t} dt = \Gamma(n+1)$$

$$S_n = \frac{2\pi^{n/2}}{\Gamma\left(\frac{n}{2}\right)}, \qquad (3)$$

$$V_n = \int_0^R S_n R^{n-1} dR = \frac{\pi^{n/2}}{\Gamma\left(\frac{n}{2}+1\right)} R^n \qquad (4)$$

For a positive integer n, $(n-1)! = \Gamma(n)$.

$$\begin{aligned}
\Gamma(\vec{r}_1, \vec{r}_2) &= \int_{q_1} \int_{q_2} e^{i\vec{q}_1 \vec{r}_1} e^{i\vec{q}_2 \vec{r}_2} \Gamma(\vec{q}_1, \vec{q}_2) \\
&= \int_{q_1} \int_{q_2} e^{i\vec{q}_1 \vec{r}_1} e^{i\vec{q}_2 \vec{r}_2} \delta(q_1 + \vec{q}_2) G(\vec{q}) \\
&= \int_q e^{i\vec{q}(\vec{r}_1 - \vec{r}_2)} G(\vec{q}) \\
&\approx \int_q e^{i\vec{q}(\vec{r}_1 - \vec{r}_2)} \frac{1}{r + q^2} \\
&\propto \frac{1}{|\vec{r}_1 - \vec{r}_2|} e^{-\sqrt{r}|\vec{r}_1 - \vec{r}_2|} \qquad (2.46)
\end{aligned}$$

in 3-dimensions. For the last step – which is not shown here – we refere the reader to the calculation of the propagator in electro-dynamics, i.e Jackson. From this result we read of

Standard Integrals

$$I_1 = \int \frac{e^{-br \pm i\,\boldsymbol{q}\bullet\boldsymbol{r}}}{r} d\boldsymbol{r} = \frac{4\pi}{b^2 + q^2};$$

$$I_2 = \int e^{-br \pm i\,\boldsymbol{q}\bullet\boldsymbol{r}} d\boldsymbol{r} = -\frac{\partial I_1}{\partial b} = \frac{8\pi b}{(b^2 + q^2)^2};$$

$$I_4 = \int \frac{e^{\pm i\,\boldsymbol{q}\bullet\boldsymbol{r}}}{|\,\boldsymbol{r} - \boldsymbol{r}'\,|} d\boldsymbol{r} = \frac{4\pi}{q^2} e^{\pm i\boldsymbol{q}\bullet\boldsymbol{r}'}$$

$$I_5 = \iint \frac{e^{-2b(r_1+r_2)}}{r_1} d\boldsymbol{r}_1 d\boldsymbol{r}_2 = \iint \frac{e^{-2b(r_1+r_2)}}{r_2} d\boldsymbol{r}_1 d\boldsymbol{r}_2 = \frac{\pi^2}{b^5}$$

$$I_6 = \iint \frac{e^{-2b(r_1+r_2)}}{r_{12}} d\boldsymbol{r}_1 d\boldsymbol{r}_2 = \frac{5\pi^2}{8b^5}, \qquad r_{12} = |\,\boldsymbol{r}_2 - \boldsymbol{r}_1\,|$$

$$I_7 = \int_{-\infty}^{\infty} \frac{e^{i\,\omega t}}{t^2 + \tau^2} dt = \frac{\pi}{\tau} e^{-\omega\tau}$$

$$I_8 = \left| \int e^{-br + i\,\omega r} dr \right|^2 = \frac{1}{b^2 + \omega^2}$$

Appendix (The Free particle-Green's function)

The solution of the equation

$$(\nabla^2 + k^2)\psi = \underbrace{u\psi}_{F(r)} \quad , \qquad (1)$$

may be written in the form

$$\psi(r) = \phi(r) + v(r) \qquad (2)$$

where $\phi(r)$ is the solution of the equation (homogeneous)

$$(\nabla^2 + k^2)\phi(r) = 0 \qquad (3)$$

using the Fourier transform of $v(r)$

$$v(r) = (2\pi)^{-\frac{3}{2}} \int A(\bar{k}') e^{i\bar{k}'\cdot\bar{r}} d^3\bar{k}' \qquad (4)$$

thus

$$F(r) = (\nabla^2 + k^2)(\phi(r) + v(r)) = (\nabla^2 + k^2) v(r) \qquad (5)$$

$$= (2\pi)^{-\frac{3}{2}} \int A(\bar{k}') (k^2 - k'^2) e^{i\bar{k}'\cdot\bar{r}} d^3k' \qquad (6)$$

where we have operated ∇^2 inside the integral

Multiplying both sides by $(2\pi)^{-\frac{3}{2}} e^{-i\bar{k}''\cdot\bar{r}}$ and integrating.

$$(2\pi)^{-\frac{3}{2}} \int F(\bar{r}) e^{-i\bar{k}''\cdot\bar{r}} d^3r = \int d^3k' (k^2 - k'^2) A(\bar{k}') \frac{1}{8\pi^3} \int e^{i(\bar{k}' - \bar{k}'')\cdot\bar{r}} d^3r$$

$$= \int d^3k' (k^2 - k'^2) A(\bar{k}') \delta(\bar{k}' - \bar{k}'')$$

or

$$A(\bar{k}'') = (2\pi)^{-\frac{3}{2}} \int F(\bar{r}) \frac{e^{-i\bar{k}''\cdot\bar{r}}}{(k^2 - k''^2)} d^3r$$

on substitution in (4), we get

$$v(\bar{r}) = \int d^3r' F(\bar{r}') G(\bar{r} - \bar{r}')$$

where

$$G(\bar{r} - \bar{r}') = -\frac{1}{8\pi^3} \int \frac{e^{ik'\cdot(\bar{r} - \bar{r}')}}{k'^2 - k^2} d^3k'$$

$$= -\frac{1}{4\pi} \frac{e^{ik|\bar{r} - \bar{r}'|}}{|\bar{r} - \bar{r}'|}$$

Notes:

1- $f(\mathbf{r}) = \int f(\mathbf{r}-\mathbf{r}')\delta(\mathbf{r}')d^3r'$

2- $G(\mathbf{r})$ is the solution of the equation: $\left(\nabla^2 \pm k^2\right)G(\mathbf{r}) = \delta(\mathbf{r})$

show that

$$\psi(r) = e^{ikz} + \int G(r, r_0)\, u(r_0)\, \psi(r_0)\, d\bar{r}_0$$

is the solution of the eq.

$$(\nabla^2 + k^2)\psi(r) = u(r)\psi(r)$$

$$(\nabla^2 + k^2)\psi(r) = (-k^2 + k^2) + \int \underbrace{(\nabla^2 + k^2)\, G(r, r_0)}_{\delta(\bar{r}-\bar{r}_0)}\, u(\bar{r}_0)\, \psi(\bar{r}_0)\, d\bar{r}_0$$

$$= 0 + \int \delta(r - r_0)\, u(r_0)\, \psi(r_0)\, d\bar{r}_0$$

$$= u(r)\psi(r)$$