Green function of a cube

Obtain the Green function satisfying the Dirichlet boundary condition inside a cube centered at the origin. Let s be the side of the cube.

Solution.
Note that the Green function $G(\mathbf{x},\mathbf{x}')$ satisfying the Dirichlet boundary condition must be symmetric in the interchange of $\mathbf{x}$ and $\mathbf{x}'$, and must vanish on the boundary. Since we are dealing with a cube, we use a Cartesian coordinate system. From Section 2.8, for a function of a single variable x,

$$\left\{1, \sqrt{\frac{2}{s}}\cos\left(\frac{2\pi n(x+s/2)}{s}\right), \sqrt{\frac{2}{s}}\sin\left(\frac{2\pi n(x+s/2)}{s}\right) : n\in\mathbb{N}\right\}$$

forms a complete orthonormal set on $I=[-s/2,s/2]$. We can generalize this to the function $G(\mathbf{x},\mathbf{x}')$ of six variables on $B=I^6$. Let $\mathbf{x}=(x,y,z)$ and $\mathbf{x}'=(x',y',z')$. Because of the boundary condition which requires that $G(\mathbf{x},\mathbf{x}')$ vanishes whenever any of $\{x,y,z,x',y',z'\}$ is at $\pm s/2$. Then the only surviving terms in the possible combinations of the orthonormal functions are the product of purely sin functions. We have the following ansatz:

$$\begin{aligned}G(\mathbf{x},\mathbf{x}') = \left(\frac{2}{s}\right)^3 \sum_{l,m,n,l',m',n'=1}^{\infty} A_{lmnl'm'n'} \sin\left(\frac{2\pi l(x+s/2)}{s}\right)\sin\left(\frac{2\pi m(y+s/2)}{s}\right)\sin\left(\frac{2\pi n(z+s/2)}{s}\right)\\ \times\sin\left(\frac{2\pi l'(x'+s/2)}{s}\right)\sin\left(\frac{2\pi m'(y'+s/2)}{s}\right)\sin\left(\frac{2\pi n'(z'+s/2)}{s}\right).\end{aligned}$$

Now, for $G(\mathbf{x},\mathbf{x}')$ to be symmetric in the interchange of $\mathbf{x}$ and $\mathbf{x}'$, we must have $l=l'$, $m=m'$, and $n=n'$. Therefore,

$$\begin{aligned}G(\mathbf{x},\mathbf{x}') = \left(\frac{2}{s}\right)^3 \sum_{l,m,n=1}^{\infty} A_{lmn} \sin\left(\frac{2\pi l(x+s/2)}{s}\right)\sin\left(\frac{2\pi m(y+s/2)}{s}\right)\sin\left(\frac{2\pi n(z+s/2)}{s}\right)\\ \times\sin\left(\frac{2\pi l(x'+s/2)}{s}\right)\sin\left(\frac{2\pi m(y'+s/2)}{s}\right)\sin\left(\frac{2\pi n(z'+s/2)}{s}\right).\end{aligned}$$

Note that $G(\mathbf{0},\mathbf{0})=0$ as expected, since the potential at the origin must also be zero by symmetry. Now, we need to normalize $G(\mathbf{x},\mathbf{x}')$ such that $\nabla'^2 G(\mathbf{x},\mathbf{x}')=-4\pi\delta(\mathbf{x}-\mathbf{x}')$. Clearly,

$$\nabla'^2 G(\mathbf{x},\mathbf{x}') = \sum_{l,m,n=1}^{\infty} -\frac{4\pi^2}{s^2}\left(l^2+m^2+n^2\right) G_{lmn}(\mathbf{x},\mathbf{x}'),$$

where

$$\begin{aligned}G_{lmn}(\mathbf{x},\mathbf{x}') = \left(\frac{2}{s}\right)^3 A_{lmn} \sin\left(\frac{2\pi l(x+s/2)}{s}\right)\sin\left(\frac{2\pi m(y+s/2)}{s}\right)\sin\left(\frac{2\pi n(z+s/2)}{s}\right)\\ \times\sin\left(\frac{2\pi l(x'+s/2)}{s}\right)\sin\left(\frac{2\pi m(y'+s/2)}{s}\right)\sin\left(\frac{2\pi n(z'+s/2)}{s}\right).\end{aligned}$$

Thus, we require

$$\sum_{l,m,n=1}^{\infty} \frac{\pi}{s^2}\left(l^2+m^2+n^2\right) G_{lmn}(\mathbf{x},\mathbf{x}') = \delta(\mathbf{x}-\mathbf{x}').$$

Using the completeness relation, we require

$$\frac{\pi}{s^2}\left(l^2+m^2+n^2\right)A_{lmn}=1,\quad \forall l,m,n\in\mathbb{N}.$$

Therefore,

$$A_{lmn}=\frac{s^2}{\pi(l^2+m^2+n^2)},$$

and the Green function is

$$G(\mathbf{x},\mathbf{x}')=\sum_{l,m,n=1}^{\infty}\frac{8}{\pi s(l^2+m^2+n^2)}\sin\left(\frac{2\pi l(x+s/2)}{s}\right)\sin\left(\frac{2\pi m(y+s/2)}{s}\right)\sin\left(\frac{2\pi n(z+s/2)}{s}\right)$$
$$\times\sin\left(\frac{2\pi l(x'+s/2)}{s}\right)\sin\left(\frac{2\pi m(y'+s/2)}{s}\right)\sin\left(\frac{2\pi n(z'+s/2)}{s}\right).$$

$\square$