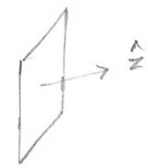
SET - 16

Free Green's function - planar geometry

1. With the goal of investigating electrostatics in materials with planar geometries,

$$\epsilon(\vec{r}) = \epsilon(z)$$



we consider

$$-\vec{\nabla} \cdot \left[\epsilon(z) \vec{\nabla} G(\vec{r}, \vec{r}\,') \right] = \delta^{(3)}(\vec{r} - \vec{r}\,')$$

2. Using the translational symmetry in x and y direction we introduce the Fourier transform

$$G(\vec{r}, \vec{r}\,') = \int_{-\infty}^{+\infty} \frac{dk_x}{2\pi} e^{ik_x(x-x')} \int_{-\infty}^{+\infty} \frac{dk_y}{2\pi} e^{ik_y(y-y')} g(z, z'; k_x, k_y)$$

$$= \int \frac{d^2k_\perp}{(2\pi)^2} e^{i\vec{k}_\perp \cdot (\vec{r} - \vec{r}\,')_\perp} g(z, z'; \vec{k}_\perp)$$

where $\vec{k}_\perp = \hat{i}\, k_x + \hat{j}\, k_y$

$$(\vec{r} - \vec{r}\,')_\perp = \hat{i}\,(x - x') + \hat{j}\,(y - y')$$

3. The Fourier transform of the δ-function in 1 is

$$\delta^{(3)}(\vec{r}-\vec{r}') = \delta(z-z') \int \frac{d^2k_\perp}{(2\pi)^2}\, e^{i\vec{k}_\perp\cdot(\vec{r}-\vec{r}')_\perp}.$$

4. Using 2 and 3 in 1 we have.

$$-\vec{\nabla}\cdot\epsilon(z)\,\vec{\nabla}\int\frac{d^2k_\perp}{(2\pi)^2}\, e^{i\vec{k}_\perp\cdot(\vec{r}-\vec{r}')_\perp}\, g(z,z';k_\perp)$$

$$= \delta(z-z')\int\frac{d^2k_\perp}{(2\pi)^2}\, e^{i\vec{k}_\perp\cdot(\vec{r}-\vec{r}')_\perp}$$

$$\int\frac{d^2k_\perp}{(2\pi)^2}\, e^{i\vec{k}_\perp\cdot(\vec{r}-\vec{r}')_\perp}\left[-\epsilon(z)\,(i\vec{k}_\perp)\cdot(i\vec{k}_\perp) - \frac{\partial}{\partial z}\epsilon(z)\frac{\partial}{\partial z}\right] g(z,z';k_\perp)$$

$$= \delta(z-z')\int\frac{d^2k_\perp}{(2\pi)^2}\, e^{i\vec{k}_\perp\cdot(\vec{r}-\vec{r}')_\perp}$$

5. Using the completeness property of Fourier functions we have.

$$\left[-\frac{\partial}{\partial z}\epsilon(z)\frac{\partial}{\partial z} + \epsilon(z)\,k_\perp^2\right] g(z,z';\vec{k}_\perp) = \delta(z-z')$$

6 Before we consider the case of $\epsilon(z)$ let us investigate the free scenario

$$\epsilon(z) = \epsilon_0 .$$

Thus,

$$-\epsilon_0 \left[\frac{\partial^2}{\partial z^2} - k_\perp^2 \right] g_0(z, z'; \vec{k}_\perp) = \delta(z - z')$$

7 For $z \neq z'$ we have

$$-\left[\frac{\partial^2}{\partial z^2} - k_\perp^2 \right] \epsilon_0\, g_0(z, z'; \vec{k}_\perp) = 0$$

which is a homogeneous differential equation with solutions $e^{-k_\perp z}$ and $e^{+k_\perp z}$.

8 The Wronskian.

$$W[e^{-k_\perp z}, e^{k_\perp z}] = \det \begin{bmatrix} e^{-k_\perp z} & e^{k_\perp z} \\ \frac{\partial}{\partial z} e^{-k_\perp z} & \frac{\partial}{\partial z} e^{k_\perp z} \end{bmatrix} = 2k_\perp,$$

being non-zero, verifies that these solutions are independent.

(9) Using (7) and (8) we can write

$$\epsilon_0 g_0(z,z';k_\perp) = \begin{cases} A e^{k_\perp z} + B e^{-k_\perp z} & z < z' \\ C e^{k_\perp z} + D e^{-k_\perp z} & z' < z \end{cases}$$

(10) Requiring the Green's function to be zero at $z=\infty$ and $z=-\infty$ we have.

$B=0$ and $C=0$.

(11) Using (10) in (9) we have

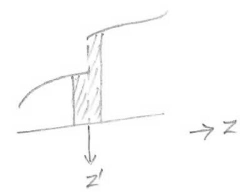
$$\epsilon_0 g_0(z,z';k_\perp) = \begin{cases} A e^{k_\perp z} & z < z' \\ D e^{-k_\perp z} & z' < z \end{cases}$$

(12) The coefficients A and D, we will show, are determined from continuity conditions on the Green's function at $z=z'$. Let us now investigate these continuity conditions.

(13) Integrating around $z = z'$ in (6) we have.

$$-\int_{z'-\delta}^{z'+\delta} dz \, \frac{\partial^2}{\partial z^2} \epsilon_0 g_0(z,z';k_\perp) + \epsilon_0 k_\perp^2 \int_{z'-\delta}^{z'+\delta} dz \, g_0(z,z';k_\perp) = 1$$

(14) Requiring g to be finite at $z = z' \pm \delta$ we have.



$$\underset{\delta \to 0}{\mathrm{Lt}} \int_{z'-\delta}^{z'+\delta} dz \, g_0(z,z';k_\perp) = 0$$

(15) Using (14) in (13) we have.

$$-\epsilon_0 \frac{\partial}{\partial z} g_0(z,z';k_\perp) \Big|_{z=z'-\delta}^{z=z'+\delta} = 1.$$

(16) Further integraty after multiplying by z is

$$-\epsilon_0 \left[z \frac{\partial^2}{\partial z^2} - z k_\perp^2 \right] g_0(z,z';k_\perp) = z \, \delta(z-z')$$

$$-\epsilon_0 \left[\frac{\partial}{\partial z} z \frac{\partial}{\partial z} - \frac{\partial}{\partial z} - z k_\perp^2 \right] g_0(z,z';k_\perp) = z \, \delta(z-z')$$

$$-\epsilon_0 \int_{z'-\delta}^{z'+\delta} dz \, \frac{\partial}{\partial z} z \frac{\partial}{\partial z} g_0(z,z';k_\perp) + \epsilon_0 \int_{z'-\delta}^{z'+\delta} dz \, \frac{\partial}{\partial z} g_0 + \epsilon_0 k_\perp^2 \underbrace{\int_{z'-\delta}^{z'+\delta} dz \, z \, g_0}_{\substack{=0 \\ \text{using (14)}}} = z'$$

(17) Thus we have.

$$- \epsilon_0 \left\{ z \frac{\partial}{\partial z} g_0(z,z';k_\perp) \right\} \Bigg|_{z=z'-\delta}^{z'+\delta} + \epsilon_0\, g_0(z,z';k_\perp) \Bigg|_{z=z'-\delta}^{z=z'+\delta} = z'$$

(18) $$\epsilon_0 \left\{ z \frac{\partial}{\partial z} g_0(z,z';k_\perp) \right\} \Bigg|_{z=z'-\delta}^{z=z'+\delta} = \epsilon_0 (z'+\delta) \left(\frac{\partial}{\partial z} g_0\right)_{z=z'+\delta} - \epsilon_0 (z'-\delta) \left(\frac{\partial}{\partial z} g_0\right)_{z=z'-\delta}$$

$$= \epsilon_0 z' \left(\frac{\partial}{\partial z} g_0\right)\Bigg|_{z=z'-\delta}^{z=z'+\delta} + \epsilon_0 \delta \left[\left(\frac{\partial}{\partial z} g_0\right)_{z=z'+\delta} + \left(\frac{\partial}{\partial z} g_0\right)_{z=z'-\delta} \right]$$

$$= z' \epsilon_0 \left(\frac{\partial g_0}{\partial z}\right) \Bigg|_{z=z'-\delta}^{z=z'+\delta} + 0$$ (requiring $\frac{\partial}{\partial z} g_0$ to be finite at $z = z' \pm \delta$.)

$$= -z'$$ (using (15)).

(19) Using (18) in (17) we have.

$$z' + \epsilon_0\, g_0(z,z';k_\perp) \Bigg|_{z=z'-\delta}^{z=z'+\delta} = z'$$

$$\epsilon_0\, g_0(z,z';k_\perp) \Bigg|_{z=z'-\delta}^{z=z'+\delta} = 0.$$

(20) Thus, we have the continuity conditions, (15) and (19),

$$\epsilon_0\, g_0(z,z';k_\perp)\Big|_{z=z'-\delta}^{z=z'+\delta} = 0$$

$$-\,\epsilon_0 \frac{\partial}{\partial z} g_0(z,z';k_\perp)\Big|_{z=z'-\delta}^{z=z'+\delta} = 1.$$

(21) Using (11) we have

$$\epsilon_0\, g_0(z,z';k_\perp) = \begin{cases} A\, e^{k_\perp z} & z<z' \\ D\, e^{-k_\perp z} & z'<z \end{cases}$$

and

$$\epsilon_0 \frac{\partial}{\partial z} g_0(z,z';k_\perp) = \begin{cases} k_\perp A\, e^{k_\perp z} & z<z' \\ -k_\perp D\, e^{-k_\perp z} & z'<z \end{cases}$$

(22) Using (21) in (20) we have.

$$D\, e^{-k_\perp z'} - A\, e^{k_\perp z'} = 0$$

$$D\, e^{-k_\perp z'} + A\, e^{k_\perp z'} = \frac{1}{k_\perp}.$$

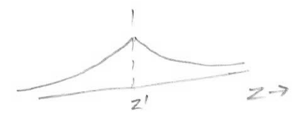
which has solutions

$$A = \frac{1}{2k_\perp} e^{-k_\perp z'} \quad \text{and} \quad D = \frac{1}{2k_\perp} e^{k_\perp z'}.$$

(23) Using (22) in (21) we have.

$$\epsilon_0 \, g_0(z,z';k_\perp) = \begin{cases} \dfrac{1}{2k_\perp} e^{-k_\perp (z'-z)} & z<z' \\ \dfrac{1}{2k_\perp} e^{-k_\perp (z-z')} & z'<z \end{cases}$$

$$= \frac{1}{2k_\perp} e^{-k_\perp |z-z'|}$$



(24) Using (23) we have a representation for free Green's function that satisfies, $\epsilon(\vec{r}) = \epsilon_0$ in (1) & (2),

$$-\epsilon_0 \nabla^2 G_0(\vec{r},\vec{r}') = \delta^{(3)}(\vec{r}-\vec{r}')$$

$$\epsilon_0 G_0(\vec{r},\vec{r}') = \int \frac{d^2k_\perp}{(2\pi)^2} e^{i\vec{k}_\perp \cdot (\vec{r}-\vec{r}')_\perp} \epsilon_0 \, g_0(z,z';k_\perp)$$

$$= \int \frac{d^2k_\perp}{(2\pi)^2} e^{i\vec{k}_\perp \cdot (\vec{r}-\vec{r}')_\perp} \frac{1}{2k_\perp} e^{-k_\perp |z-z'|}.$$

(25) The above representation is, of course, equal to

$$\epsilon_0 G_0(\vec{r},\vec{r}') = \frac{1}{4\pi} \frac{1}{|\vec{r}-\vec{r}'|}.$$