We derive the solutions to the Schrödinger equation in a 3D box of sidelength L with periodic boundary conditions.

The TISE is given by

$$-\frac{\hbar^2}{2m}\nabla^2\Psi = E\Psi$$

We now separate variables: $\Psi(x,y,z) = X(x)Y(y)Z(z)$

$$\Rightarrow -\frac{\hbar^2}{2m}\nabla^2\Psi = -\frac{\hbar^2}{2m}(\partial_{xx}+\partial_{yy}+\partial_{zz})\,X(x)Y(y)Z(z)$$

$$= -\frac{\hbar^2}{2m}\left[X''(x)Y(y)Z(z) + X(x)Y''(y)Z(z) + X(x)Y(y)Z''(z)\right]$$

$$= E\,X(x)Y(y)Z(z) \Rightarrow$$

$$\frac{X''(x)}{X(x)} + \frac{Y''(y)}{Y(y)} + \frac{Z''(z)}{Z(z)} = -\frac{2mE}{\hbar^2}$$

We observe that each term on the LHS depends on a different variable, and also that the RHS is constant. To keep the RHS constant, it is impossible to vary one of the functions without varying the others. However, since the functions all depend on different arguments, it must be impossible to vary any of them.

Thus, each term on the LHS must be a constant. We choose a negative real constant for each, in order to preserve periodic BCs.

$$\frac{X''(x)}{X(x)} = -k_x^2, \quad \frac{Y''(y)}{Y(y)} = -k_y^2, \quad \frac{Z''(z)}{Z(z)} = -k_z^2$$

The RHS implies that $E = \hbar^2/2m \, (k_x^2 + k_y^2 + k_z^2)$. Solving each of these, we have

$$f''(a) = -k_a^2 f(a) \implies f(a) = Ae^{ik_a \cdot a} + Be^{-ik_a a} \implies$$

$$f'(a) = k_a \cdot a \cdot \left(A\, e^{ik_a \cdot a} - Be^{-ik_a a}\right).$$

We now plug boundary conditions into f, f': $f(0) = f(L) \implies$

$$A + B = Ae^{ik_a L} + Be^{-ik_a L}. \quad f'(0) = f'(L) \implies$$

$$A - B = Ae^{ik_a L} - Be^{-ik_a L} \implies 2A = 2Ae^{ik_a L} \implies$$

$$k_a L = 2 n_a \pi, \; n_a \in \mathbb{Z} \implies k_a = 2 n_a \pi / L, \; n_a \in \mathbb{Z}.$$

Thus, our solutions are plane waves $1/\sqrt{V} \cdot e^{i\vec{k}\cdot\vec{x}}$ (normalization is trivial to check), and we have $k_x = 2n_x\pi/L$, $k_y = 2n_y\pi/L$, $k_z = 2n_z\pi/L$; $n_x, n_y, n_z \in \mathbb{Z}$, and $E = \frac{\hbar^2 \vec{k}^2}{2m} = \frac{4\pi^2\hbar^2}{2mL^2}\left(n_x^2 + n_y^2 + n_z^2\right)$.