Square lattice *Consider a square lattice in two dimensions with the crystal potential:*

$$U(x,y) = -4U\cos(2\pi x/a)cos(2\pi y/a). \tag{16}$$

By using Fourier analysis in 2D, find approximately the energy gap (E_g) at the corner *point* $(\pi/a, \pi/a)$ *of the Brillouin zone.*

As described in Problem 1 of this set and as you know by now anyway, the square crystal lattice has a reciprocal lattice that is also square. The first Brillouin zone is a square of side $2\pi/a$. We need to know the components of the Fourier series for $U(x,y)$. These can be found directly by integration of $U(x,y)e^{-i\vec{k}\cdot(x,y)}$ or by noting that

$$\begin{aligned}
U(x,y) &= -4U\cos(2\pi x/a)\cos(2\pi y/a) & (17)\\
&= -U\left[2\cos(2\pi x/a)\right]\left[2\cos(2\pi y/a)\right] & (18)\\
&= -U\left(e^{2\pi x/a}+e^{-2\pi x/a}\right)\left(e^{2\pi y/a}+e^{-2\pi y/a}\right) & (19)\\
&= -U\left(e^{2\pi x/a+2\pi y/a}+e^{2\pi x/a-2\pi y/a}+e^{-2\pi x/a+2\pi y/a}+e^{-2\pi x/a-2\pi y/a}\right) & (20)\\
&= -U\left(e^{i\vec{G}_{++}\cdot\vec{x}}+e^{i\vec{G}_{+-}\cdot\vec{x}}+e^{i\vec{G}_{-+}\cdot\vec{x}}+e^{i\vec{G}_{--}\cdot\vec{x}}\right) & (21)\\
&= \sum_{\vec{G}} C_{\vec{G}}e^{i\vec{G}\cdot\vec{x}} & (22)
\end{aligned}$$

$\vec{G}_{\pm\pm} = \pm\frac{2\pi}{a}\hat{x} \pm \frac{2\pi}{a}\hat{y}$ and $C_{\vec{G}} = -U$ for $\vec{G} = \vec{G}_{\pm\pm}$ and $C_{\vec{G}} = 0$ for all other $\vec{G}$.

Thus $\vec{k} = \left(\frac{\pi}{a}, \frac{\pi}{a}\right)$ corresponds to the corner on the first Brillouin zone (1st B.Z.) where Bragg scattering of electron waves can occur if the following Bragg condition is fulfilled:

$$2\vec{k}\cdot\vec{G} = G^2 \quad \Rightarrow \quad \vec{k}\cdot\frac{1}{2}\vec{G} = \left(\frac{G}{2}\right)^2 \Rightarrow \vec{k}\cdot\hat{G}_i = G_i/2$$

$$\vec{k}\cdot\hat{G}_{++} = \left(\frac{\pi}{a}, \frac{\pi}{a}\right)\cdot\left(\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}\right) = \frac{\pi}{a}\sqrt{2} = \frac{1}{2}\left|\vec{G}_{++}\right| = \frac{1}{2}\frac{2\pi}{a}\sqrt{2}$$

Thus, because $\boldsymbol{G}_{++}$ fulfills this condition and is one of the four reciprocal lattice vectors in the Fourier series of the crystal potential, the band gap (E_g) is two times the magnitude of the Fourier coefficient that corresponds to $\boldsymbol{G}_{++}$ and is $E_g = 2|C_{\boldsymbol{G}++}| = 2|U|$.