Problem 1. (a) From Kittel, for a periodic delta-function potential we get the simplified equation

$$\frac{P}{Ka}\sin(Ka) + \cos(Ka) = \cos(ka)$$

where $\cos(ka) = 1$ at $k = 0$. Taking the Taylor series approximations for small Ka:

$$\sin(Ka) = Ka \dots$$
$$\cos(Ka) = 1 - \frac{1}{2}(Ka)^2 + \dots$$

but if we approximate only to the first order, we get

$$\frac{P}{Ka}Ka + 1 = 1 \implies P = 0$$

which doesn't tell us any information to find the band gap

$$\epsilon = \frac{\hbar^2 K^2}{2m}$$

so we take the second order approximation for the cosine term:

$$\frac{P}{Ka}Ka + 1 - \frac{1}{2}(Ka)^2 = 1$$
$$\implies K^2 = \frac{2P}{a^2}$$

so the band gap is

$$\epsilon \approx \frac{\hbar^2 P}{ma^2}$$

(b) For $k = \pi/a$, $\cos ka = -1$ and the equation becomes

$$\frac{P}{Ka}\sin(Ka) + \cos(Ka) = -1$$

and from Figure 1 we can approximate the Taylor series around $Ka = \pi + h$:

$$f(x+h) \approx f(x) + hf'(x) + \frac{1}{2}h^2 f''(x)$$

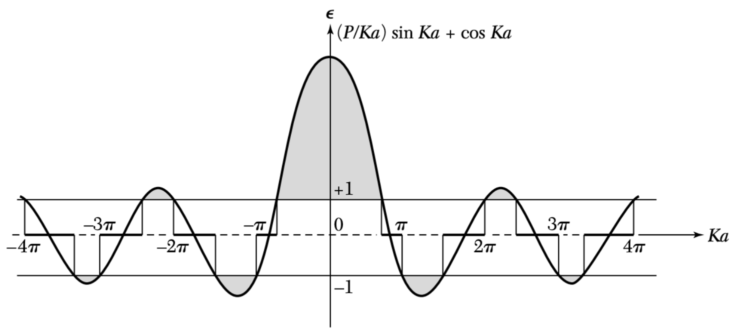

Figure 1: From Kittel

so we have

$$\sin(Ka) \approx \sin\pi + h\cos\pi = -h$$
$$\cos(Ka) \approx \cos\pi + h(-\sin\pi) + \frac{1}{2}h^2(-\cos\pi) = -1 + \frac{1}{2}h^2$$

and thus

$$\frac{P}{\pi}(-h) + \left(-1 + \frac{1}{2}h^2\right) = -1$$
$$\implies h = \frac{2P}{\pi}$$

where

$$(Ka)^2 = (\pi + h)^2 = \pi^2 + 2\pi h + h^2$$
$$\implies K^2 = \frac{\pi^2 + 2\pi h}{a^2} = \frac{\pi^2 + 4P}{a^2}$$

so the band gap is

$$\epsilon \approx \frac{\hbar^2 K^2}{2ma^2} = \frac{\hbar^2}{2ma^2}\frac{\pi^2 + 4P}{a^2}$$

Problem 2 Using the central equation

$$(\lambda_k - \epsilon)C(k) + \sum_G U_G C(k - G) = 0$$

where the energy gap occurs at

$$k = \pm\frac{\pi}{a}\hat{\mathbf{x}} + \pm\frac{\pi}{a}\hat{\mathbf{y}}$$

and from the Bragg condition $(\mathbf{k} + \mathbf{G})^2 = k^2$ the reciprocal lattice vector is

$$G = \frac{2\pi}{a}\hat{\mathbf{x}} + \frac{2\pi}{a}\hat{\mathbf{y}}$$

using the relation $k - G = -\frac{\pi}{a}$ we have two equations to solve for the energy gap:

$$(\lambda - \epsilon)C\left(\frac{\pi}{a}, \frac{\pi}{a}\right) + U_G C\left(-\frac{\pi}{a}, -\frac{\pi}{a}\right) = 0$$
$$(\lambda - \epsilon)C\left(-\frac{\pi}{a}, -\frac{\pi}{a}\right) + U_G C\left(\frac{\pi}{a}, \frac{\pi}{a}\right) = 0$$

which can be written as a matrix equation

$$\begin{pmatrix} \lambda - \epsilon & U_G \\ U_G & \lambda - \epsilon \end{pmatrix} \begin{pmatrix} C\left(\frac{\pi}{a}, \frac{\pi}{a}\right) \\ C\left(-\frac{\pi}{a}, -\frac{\pi}{a}\right) \end{pmatrix} = 0$$

so the determinant of the matrix is

$$(\lambda - \epsilon)^2 - U_G^2 = 0$$
$$\implies \epsilon = \lambda \pm U_G$$

and thus the two roots tells us that the energy gap is $E_g = 2|U_G|$. From the Fourier transform of the potential:

$$U = \sum_G U_G e^{i\mathbf{G}\cdot\mathbf{r}}$$
$$U(x, y) = \sum_G U_G \cos(G_x x)\cos(G_y y)$$

so the fourier coefficients of the potential is

$$\begin{aligned} U_G &= \iint_0^a U(x, y)\cos(G_x x)\cos(G_y y)\,\mathrm{d}x\,\mathrm{d}y \\ &= \iint_0^a U(x, y)\cos\left(\frac{2\pi x}{a}\right)\cos\left(\frac{2\pi y}{a}\right)\mathrm{d}x\,\mathrm{d}y \\ &= 4U\frac{4}{a^2}\iint_0^a \cos^2\left(\frac{2\pi x}{a}\right)\cos^2\left(\frac{2\pi y}{a}\right)\mathrm{d}x\,\mathrm{d}y \end{aligned}$$

where

$$\int_0^a \cos^2\left(\frac{2\pi x}{a}\right) \mathrm{d}x = \frac{a}{2}$$

so

$$U_G = -4U\frac{4}{a^2}\left(\frac{a}{2}\frac{a}{2}\right) = -4U$$

and the magnitude of the band gap is

$$E_g = 2|U_G| = 8U$$