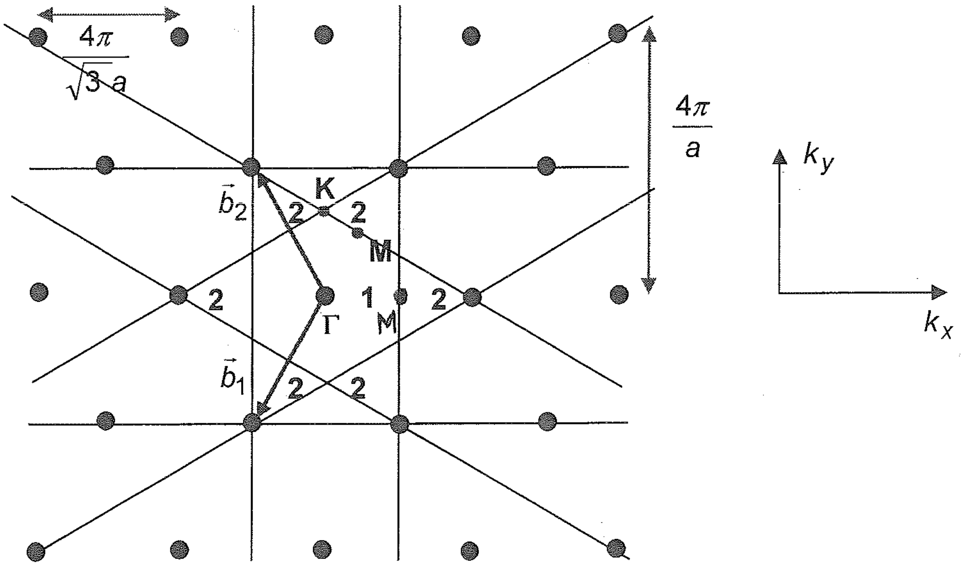
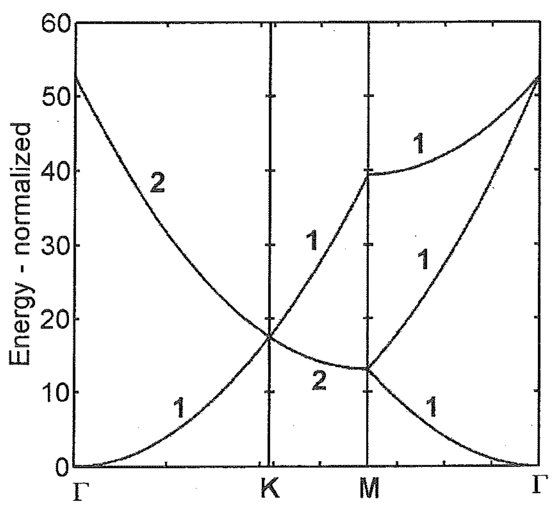
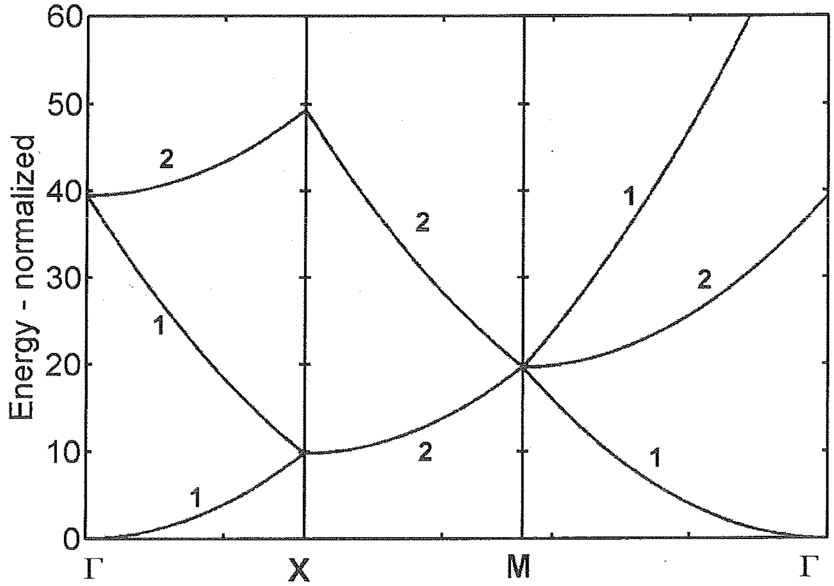


4.1: (a) and (b)



Bandgaps can open up at the K and M points

4.2: (a)



4.2

a) See attached

b) $\vec{k} = \left(-\frac{\pi}{a}, 0\right)$

c) $\vec{k} = \left(0, -\frac{\pi}{a}\right)$

d) $\vec{k} = \left(\frac{\pi}{a}, -\frac{\pi}{a}\right)$ $\quad \vec{k} = \left(-\frac{\pi}{a}, \frac{\pi}{a}\right)$ $\quad \vec{k} = \left(-\frac{\pi}{a}, \frac{\pi}{a}\right)$

e) $|\psi_{(\frac{\pi}{a},0)}\rangle = c_1 |\phi_{(\frac{\pi}{a},0)}\rangle + c_2 |\phi_{(-\frac{\pi}{a},0)}\rangle$

Matrix is:

$$\begin{bmatrix} e\left(\frac{\pi}{a},0\right)+V_0 & \frac{V_1}{2} \\ \frac{V_1}{2} & V_0 + e\left(-\frac{\pi}{a},0\right) \end{bmatrix} \begin{bmatrix} c_1 \\ c_2 \end{bmatrix} = E\left(\frac{\pi}{a},0\right) \begin{bmatrix} c_1 \\ c_2 \end{bmatrix}$$

where $e\left(\frac{\pi}{a},0\right) = \frac{\hbar^2}{2m}\left(\frac{\pi}{a}\right)^2 = e\left(-\frac{\pi}{a},0\right)$

Solution is:

$$E_\pm\left(\frac{\pi}{a},0\right) = e\left(\frac{\pi}{a},0\right) + V_0 \pm \frac{|V_1|}{2}$$

$$\begin{bmatrix} c_1 \\ c_2 \end{bmatrix}_+ = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ 1 \end{bmatrix} \qquad \begin{bmatrix} c_1 \\ c_2 \end{bmatrix}_- = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ -1 \end{bmatrix}$$

$$\Rightarrow \psi_{(\frac{\pi}{a},0)}(x,y) = \begin{cases} \sqrt{\frac{2}{A}} \cos\left(\frac{\pi}{a}x\right) & \leftarrow \text{higher energy sol.} \\ i\sqrt{\frac{2}{A}} \sin\left(\frac{\pi}{a}x\right) & \leftarrow \text{lower energy sol.} \end{cases}$$

f) $|\psi_{(0,\frac{\pi}{a})}\rangle = c_1 |\phi_{(0,\frac{\pi}{a})}\rangle + c_2 |\phi_{(0,\frac{\pi}{a})}\rangle$

Matrix is:

$$\begin{bmatrix} e\left(0,\frac{\pi}{a}\right)+V_0 & \frac{V_2}{2} \\ \frac{V_2}{2} & e\left(0,-\frac{\pi}{a}\right)+V_0 \end{bmatrix} \begin{bmatrix} c_1 \\ c_2 \end{bmatrix} = E\left(0,\frac{\pi}{a}\right) \begin{bmatrix} c_1 \\ c_2 \end{bmatrix}$$

Solution is :

$$E_\pm\left(0,\frac{\pi}{a}\right) = e\left(0,\frac{\pi}{a}\right) + V_0 \pm \frac{|V_2|}{2}$$

$$\begin{bmatrix} c_1 \\ c_2 \end{bmatrix}_+ = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ 1 \end{bmatrix} \qquad \begin{bmatrix} c_1 \\ c_2 \end{bmatrix}_- = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ -1 \end{bmatrix}.$$

$$\psi_{(0,\frac{\pi}{a})}(x,y) = \begin{cases} \sqrt{\frac{2}{A}}\cos\left(\frac{\pi}{a}y\right) & \longleftarrow \text{higher energy sol.} \\ i\sqrt{\frac{2}{A}}\sin\left(\frac{\pi}{a}y\right) & \longleftarrow \text{lower energy sol.} \end{cases}$$

g) $|\psi_{(\frac{\pi}{a},\frac{\pi}{a})}\rangle = c_1|\phi_{(\frac{\pi}{a},\frac{\pi}{a})}\rangle + c_2|\phi_{(-\frac{\pi}{a},\frac{\pi}{a})}\rangle + c_3|\phi_{(\frac{\pi}{a},-\frac{\pi}{a})}\rangle$

$$+ c_4|\phi_{(-\frac{\pi}{a},-\frac{\pi}{a})}\rangle.$$

Matrix is:

$$\begin{bmatrix} e_0+V_0 & V_1/2 & V_2/2 & V_3/2 \\ V_1/2 & e_0+V_0 & V_3/2 & V_2/2 \\ V_2/2 & V_3/2 & e_0+V_0 & V_1/2 \\ V_3/2 & V_2/2 & V_1/2 & e_0+V_0 \end{bmatrix}\begin{bmatrix} c_1 \\ c_2 \\ c_3 \\ c_4 \end{bmatrix} = E\left(\frac{\pi}{a},\frac{\pi}{a}\right)\begin{bmatrix} c_1 \\ c_2 \\ c_3 \\ c_4 \end{bmatrix}.$$

where $e_0 = e\left(\frac{\pi}{a},\frac{\pi}{a}\right) = \frac{\hbar^2}{2m}\left[\left(\frac{\pi}{a}\right)^2+\left(\frac{\pi}{a}\right)^2\right].$

Solutions are:

1) $E\left(\frac{\pi}{a},\frac{\pi}{a}\right) = e_0+V_0 + \left(\frac{V_1+V_2+V_3}{2}\right)$ $\qquad \begin{bmatrix} c_1 \\ c_2 \\ c_3 \\ c_4 \end{bmatrix} = \frac{1}{2}\begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix}$

2) $E\left(\frac{\pi}{a},\frac{\pi}{a}\right) = e_0+V_0 + \left(\frac{V_1-V_2-V_3}{2}\right)$ $\qquad \begin{bmatrix} c_1 \\ c_2 \\ c_3 \\ c_4 \end{bmatrix} = \frac{1}{2}\begin{bmatrix} 1 \\ 1 \\ -1 \\ -1 \end{bmatrix}.$

3) $E(\frac{\pi}{a},\frac{\pi}{a}) = e_0 + V_0 + \left(\frac{-V_1 + V_2 - V_3}{2}\right)$ $\quad \begin{bmatrix} c_1 \\ c_2 \\ c_3 \\ c_4 \end{bmatrix} = \frac{1}{2}\begin{bmatrix} -1 \\ 1 \\ -1 \\ 1 \end{bmatrix}$.

4) $E(\frac{\pi}{a},\frac{\pi}{a}) = e_0 + V_0 + \left(\frac{-V_1 - V_2 + V_3}{2}\right)$ $\quad \begin{bmatrix} c_1 \\ c_2 \\ c_3 \\ c_4 \end{bmatrix} = \frac{1}{2}\begin{bmatrix} 1 \\ -1 \\ -1 \\ 1 \end{bmatrix}$.

wavefunctions are:

1) $\psi_{(\frac{\pi}{a},\frac{\pi}{a})}(x,y) = \sqrt{\frac{4}{A}} \cos(\frac{\pi}{a}x)\cos(\frac{\pi}{a}y)$.

2) $\psi_{(\frac{\pi}{a},\frac{\pi}{a})}(x,y) = i\sqrt{\frac{4}{A}} \cos(\frac{\pi}{a}x)\sin(\frac{\pi}{a}y)$.

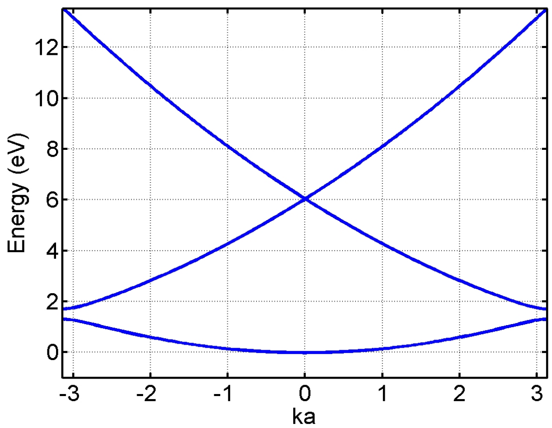
3) $\psi_{(\frac{\pi}{a},\frac{\pi}{a})}(x,y) = -i\sqrt{\frac{4}{A}} \sin(\frac{\pi}{a}x)\cos(\frac{\pi}{a}y)$.

4) $\psi_{(\frac{\pi}{a},\frac{\pi}{a})}(x,y) = -\sqrt{\frac{4}{A}} \sin(\frac{\pi}{a}x)\sin(\frac{\pi}{a}y)$.

h) The degeneracy at the M-point has been lifted provided $|V_1| \neq |V_2|$. Otherwise two bands will still be degenerate at the M-point.

4.3:

a) See plot below.



a) V_1=0.2 eV and V_2 = 0.0 eV

b) The size of the bandgap that opens at ka=±π is approximately 0.4 eV which equals $2V_1$ as predicted by the nearly free electron model.

c) See the matrix given below for this part.

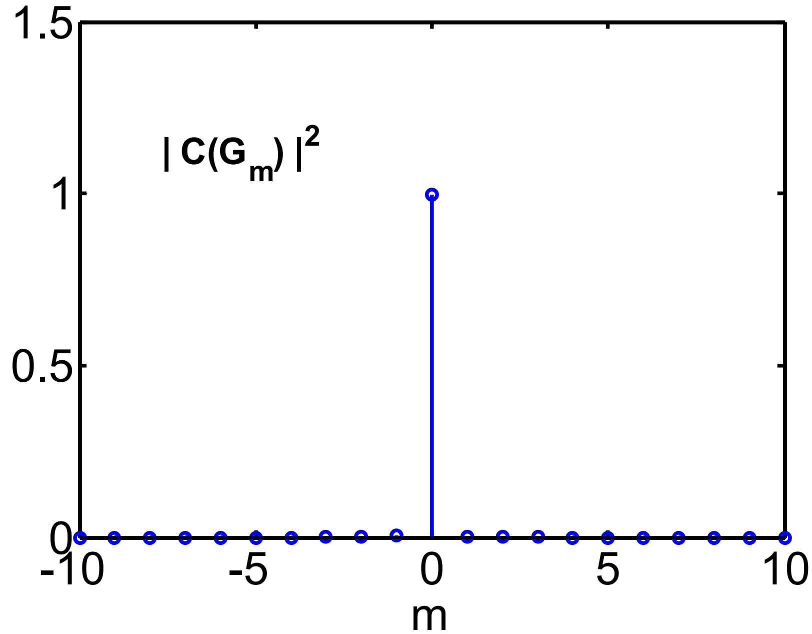
$$\begin{bmatrix} \ddots & & & & & & \\ & e(k+G_{-2}) & V_1 & V_2 & & & \\ & V_1 & e(k+G_{-1}) & V_1 & V_2 & & \\ & V_2 & V_1 & e(k) & V_1 & V_2 & \\ & & V_2 & V_1 & e(k+G_1) & V_1 & \\ & & & V_2 & V_1 & e(k+G_2) & \\ & & & & & & \ddots \end{bmatrix} \begin{bmatrix} \vdots \\ c(G_{-2}) \\ c(G_{-1}) \\ c(0) \\ c(G_{-1}) \\ c(G_{-2}) \\ \vdots \end{bmatrix}$$

$$= E(k) \begin{bmatrix} \vdots \\ c(G_{-2}) \\ c(G_{-1}) \\ c(0) \\ c(G_{-1}) \\ c(G_{-2}) \\ \vdots \end{bmatrix}$$

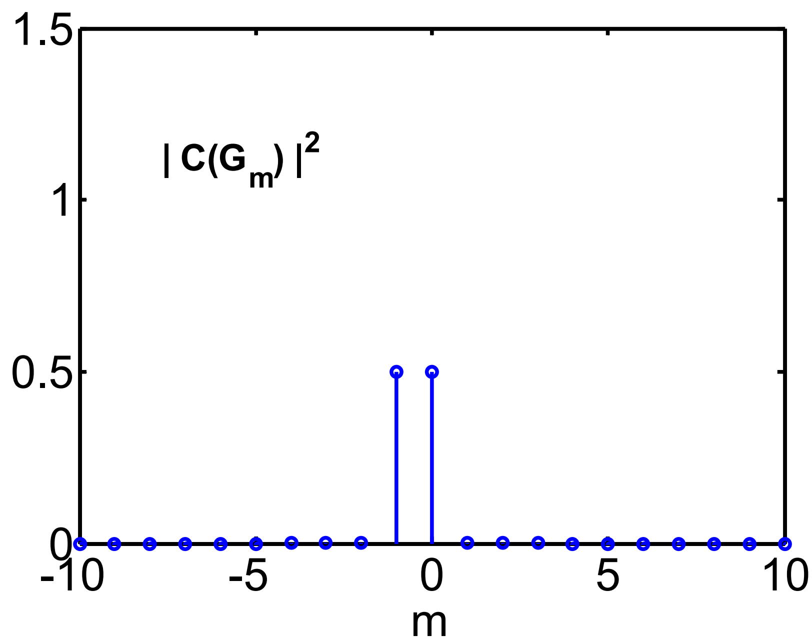
d) See the plot attached below.

e) See the plot attached below. The result is as expected because the plane wave solution at the Bragg point gets strongly coupled with (or mixed with) its Bragg scattering counterpart(s).

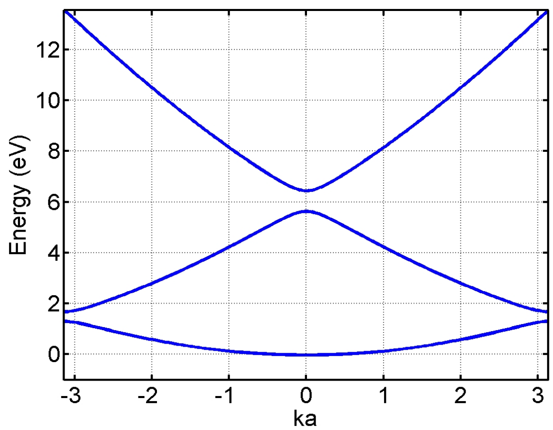
d)



e)



f) and g) and h) See answer to part (c) for part (f) answer.



d) V_1=0.2 eV and V_2 = 0.4 eV

The bandgaps now open at ka=0 between the second and the third energy band – of magnitude ~0.8 eV – and at ka=±π between the first and the second energy band – of magnitude ~0.4 eV. The values of the bandgaps are in decent agreement with the nearly free electron model.

i) See attached plot

i)