HW 2 Solutions

1) 2 atoms per basis because you need a basis of 2 atoms to place at each lattice point in order to arrive at the hexagonal structure.

2) Area is given by the area enclosed by the two lattice vectors \( \vec{a}_1 \) and \( \vec{a}_2 \) and using this idea we get

\[
A = \frac{3\sqrt{3}}{2} a^2
\]

2 \times \left( \frac{a}{2} \times 3 \right) \times \left( \frac{a}{2} \times 2\sqrt{3} \right) \times \frac{1}{2}

\[\text{base} \hspace{1cm} \text{height}\]

3) I will take a slightly different approach here and look for \( b_1 \) and \( b_2 \) so that they satisfy \( \vec{a}_i \cdot \vec{b}_j = 2\pi \delta_{ij} \)

\[
\vec{a}_1 = \frac{a}{2} (3, \sqrt{3}) \quad \vec{a}_2 = \frac{a}{2} (3, -\sqrt{3})
\]

\[
\begin{align*}
\vec{a}_1 \cdot \vec{b}_1 & = \frac{3a}{2} b_1 + \frac{\sqrt{3}a}{2} b_2 = 2\pi \\
\vec{a}_2 \cdot \vec{b}_1 & = \frac{3a}{2} b_1 - \frac{\sqrt{3}a}{2} b_2 = 0
\end{align*}
\]

\[
\begin{align*}
\vec{a}_1 \cdot \vec{b}_2 & = \frac{3a}{2} b_2 + \frac{\sqrt{3}a}{2} b_2 = 2\pi \\
\vec{a}_2 \cdot \vec{b}_2 & = \frac{3a}{2} b_2 - \frac{\sqrt{3}a}{2} b_2 = 0
\end{align*}
\]

\[
\begin{align*}
b_1 & = \frac{2\pi}{\sqrt{3}} a \\
b_2 & = \frac{2\pi}{a \sqrt{3}}
\end{align*}
\]
like wise for $b_2 = (b_1, b_2)$

\[
\begin{align*}
\alpha_1 \cdot b_2 &= \frac{3\alpha}{2} b_1 + \frac{\sqrt{3} \alpha}{2} b_2 = 0 \\
\alpha_2 \cdot b_2 &= \frac{3\alpha}{2} b_1 - \frac{\sqrt{3} \alpha}{2} b_2 = 2\pi
\end{align*}
\]

Add these two together to get

\[
3\alpha b_1 = 2\pi \Rightarrow b_1 = \frac{2\pi}{\alpha} \frac{1}{3}
\]

Now plug this back into the first equation to get:

\[
\frac{3\alpha}{2} b_1 \left( \frac{2\pi}{\alpha} \cdot \frac{1}{3} \right) + \frac{\sqrt{3} \alpha}{2} b_2 = 0
\]

\[
71 + \frac{\sqrt{3} \alpha}{2} b_2 = 0 \\
\Rightarrow b_2 = -\frac{2\pi}{\alpha} \frac{1}{\sqrt{3}}
\]

Note that I used $b_2 = (b_1, b_2)$ as a convenient notation.

Finally we get $b_1 = \frac{2\pi}{\alpha} \left( \frac{1}{3}, 1, \frac{1}{\sqrt{3}} \right)$

and $b_2 = \frac{2\pi}{\alpha} \left( \frac{1}{3}, 1, -\frac{1}{\sqrt{3}} \right)$
d) The 1st pz has 6 corners, each shared by 3 neighboring zones so 2 unique corners per zone.

f) Usually we pick the 2 corners enclosed by the lattice vectors as the unique choice. Their kx coordinates are the same as the kx component of b₁ and b₂, and their ky location is 1/3 of the way up, so:

\[ K = \frac{2\pi}{a} \left( \frac{1}{3}, \frac{1}{3\sqrt{3}} \right), \quad K' = \frac{2\pi}{a} \left( \frac{1}{3}, \frac{-1}{3\sqrt{3}} \right) \]

\[ E(0) = \pm tv_f |K-K'| \]

\[ \nabla E(0) = \pm tv_f \frac{(K' - K)}{|K' - K|} \Rightarrow |\nabla E(0)| = tv_f \]

\[ L(E) = 2\pi |\vec{K}-\vec{K}'| = \frac{2\pi}{tv_f} |E| \text{ since the length of the constant energy contour is always positive.} \]
\[ D(E) = \frac{1}{(2\pi)^2} \cdot \frac{|E|}{h v_F}, \quad 2\pi \cdot \frac{1}{k v_F} \]

\[ = \frac{|E|}{2\pi h^2 v_F^2} \]

If we include spin degeneracy of 2 this becomes \( D(E) = \frac{|E|}{\pi h^2 v_F^2} \).

If we wanted the DOS per unit cell, then we would multiply this result, which is per unit area, by the area of the unit cell and by a factor of 2 for 2 atoms per basis (i.e., per unit cell).

\[ D(E) \]

\[ \frac{1}{\pi h^2 v_F^2} \]

\( E \)

b) \( V_g(\mathbf{k}^2) = \frac{1}{4} \nabla_k E(\mathbf{k}) = \pm v_F \frac{1}{|\mathbf{k} - \mathbf{k}'|} \) since the group velocity is a vector pointing in the direction of \( \mathbf{k} - \mathbf{k}' \) with length \( v_F \).
2) a) 
\[ E(k) = \frac{\hbar^2}{2m^*} \left( k_x^2 + k_y^2 \right) \]

b) The constant energy contour is a circle of radius \( |k| = \sqrt{k_x^2 + k_y^2} \)
\[ S(k_x, k_y) = 2\pi |k| \]

c) 
\[ S(E) = 2\pi \sqrt{\frac{2m^*}{\hbar^2} E} \]
Because \( |k| = \sqrt{k_x^2 + k_y^2} = \sqrt{\frac{2m^*}{\hbar^2} E} \)

d) \[ \Delta E = \frac{\hbar^2}{2m^*} (2k_x, 2k_y) \]
\[ |\Delta E| = \frac{\hbar^2}{m^*} |k| = \frac{\hbar^2}{m^*} \sqrt{\frac{2m^*}{\hbar^2} E} \]

e) \[ g(E) = \frac{1}{(2\pi)^2} \frac{S(E)}{|\Delta E|} = \frac{1}{(2\pi)^2} \frac{2\pi |k|}{\frac{\hbar^2}{m^*} \sqrt{\frac{2m^*}{\hbar^2} E}} \]

OR using \[ g(E) = \frac{1}{(2\pi)^2} \frac{\frac{2m^*}{\hbar^2} E}{\frac{\hbar^2}{m^*} \sqrt{\frac{2m^*}{\hbar^2} E}} \]
\[ = \frac{m^*}{2\pi \hbar^2} \]

Note: Since electrons have spin up and spin down, there are two electrons per site, so \( 2d \) \( g(E) \) is often given as \( g(E) = \frac{m^*}{\pi \hbar^2} \).
$E(k) = \alpha |k|^{3/2}$

$|k| = \sqrt{\frac{E}{\alpha}}$

$|\nabla E(k)| = \alpha \beta |k|^{\beta-1} = 2\beta |\frac{E}{\alpha}|^{\frac{\beta-1}{\beta}}$

$= \alpha^{1/\beta} \beta^{-1/\beta} E$

$A(E) = 4\pi |\frac{E}{\alpha}|^2 = 4\pi |\frac{E}{\alpha}|^{2/\beta}$

$D(E) = \frac{1}{(2\pi)^3} \cdot A(E) \cdot \frac{1}{1|\nabla E|}$

$= \frac{1}{2\pi^2} \frac{E^{2/\beta}}{2^{2/\beta}} \left[ \alpha^{1/\beta} \beta^{-1/\beta} E^{1-1/\beta} \right]$

$= \frac{1}{2\pi^2} \frac{1}{\alpha^{3/\beta}} \cdot E^{\frac{2}{\beta} - 1} + \frac{1}{\beta}$

$= \frac{1}{2\pi^2} \frac{E}{\alpha^{3/\beta}}$

For $\beta = 2$ (quadratic), we get $D(E) dE^{1/2}$ which matches the DOS of electrons.

For $\beta = 1$ (linear phonons), we get that $D(E) \propto \frac{E}{\alpha^3}$ which matches the phonon DOS.