1) a) \( \hat{a}_1 = a \hat{x} \quad \hat{a}_2 = \frac{a}{2} (-\hat{x} + \sqrt{3} \hat{y}) \quad \hat{a}_3 = c \hat{z} \)

\[
\begin{array}{c}
\hat{a}_1 - \hat{a}_2 - \hat{a}_3 \rightarrow \hat{x} \\
\end{array}
\]

b) \( V = \hat{a}_1 \cdot (\hat{a}_2 \times \hat{a}_3) = \hat{a}_2 \cdot (\hat{a}_3 \times \hat{a}_1) = \hat{a}_3 \cdot (\hat{a}_1 \times \hat{a}_2) \)

This one is easiest because \( \hat{a}_1 \) and \( \hat{a}_3 \) are orthogonal so \( \hat{a}_1 \times \hat{a}_3 = ac \hat{\gamma} \)

\[
V = \hat{a}_1 \cdot (ac \hat{\gamma}) = \frac{a^2 c}{2} (-\hat{x} + \sqrt{3} \hat{y}) \cdot \hat{\gamma} = \frac{\sqrt{3}}{2} a^2 c
\]

Could also use base x height for the slope.

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

Then multiply "leg the height " \( c \) of the primitive unit cell to get:

\[
V = \frac{\sqrt{3}}{2} a^2 c
\]
c) 
\[ \mathbf{b}_1 = \frac{2\pi}{V} (\mathbf{\hat{a}}_2 \times \mathbf{\hat{a}}_3) = \frac{2\pi}{V} \frac{a c}{2} \left[ (\mathbf{\hat{x}} \times \mathbf{\hat{y}}) \times \mathbf{\hat{z}} \right] \]
\[ = \frac{2\pi}{\sqrt{3} a} (\mathbf{\hat{y}} \times \mathbf{\hat{z}}) \]
\[ \mathbf{b}_2 = \frac{2\pi}{V} (\mathbf{\hat{a}}_3 \times \mathbf{\hat{a}}_1) = \frac{2\pi}{V} ac \mathbf{\hat{y}} \]
\[ = \frac{4\pi}{\sqrt{3} a} \mathbf{\hat{y}} \]
\[ \mathbf{b}_3 = \frac{2\pi}{V} (\mathbf{\hat{a}}_1 \times \mathbf{\hat{a}}_2) = \frac{2\pi}{V} \frac{a^2}{2} \left[ (\mathbf{\hat{x}} \times (\mathbf{\hat{x}} \times \mathbf{\hat{y}})) \right] \]
\[ = \frac{4\pi}{\sqrt{3} c} \cdot \frac{\sqrt{3}}{2} \mathbf{\hat{x}} \mathbf{\hat{z}} = \frac{2\pi}{c} \mathbf{\hat{x}} \]

d)

\[ e) \quad \text{The lattice structure in reciprocal space is also hexagonal.} \]
2 a) Path difference is 0
for $\theta = 0^\circ$ and $2d$ for $\theta = 90^\circ$
so $2d \sin \theta$ (also based on
the figure)

b) The path difference has to
be a multiple of a wave length
so \( n \lambda = 2d \sin \theta \) for \( n = 1, 2, 3, \ldots \)

c) 
\[
\begin{align*}
\hat{\mathbf{r}} &= |\mathbf{r}| - \mathbf{r} \\
\hat{\mathbf{r}}' &= |\mathbf{r}'| - \mathbf{r}'
\end{align*}
\]
and \( |\mathbf{r}| = |\mathbf{r}'| \) so
\[
k - k' = |\mathbf{r}| - 2 \sin \theta = \frac{2\pi}{\lambda} 2 \sin \theta
\]
\[
G = n \cdot \frac{2\pi}{d}
\]
so
\[
\frac{2\pi}{\lambda} 2 \sin \theta = n \frac{2\pi}{d}
\]
\[
\Rightarrow 2d \sin \theta = n \lambda
\]
OR
\[
\hat{\mathbf{r}}_\parallel = \hat{\mathbf{r}}'_\parallel \quad \text{and} \quad \hat{\mathbf{r}}_\perp - \hat{\mathbf{r}}'_\perp = (|\mathbf{r}| 2 \sin \theta)
\]
\[
= \frac{2\pi}{\lambda} 2 \sin \theta = n \frac{2\pi}{d}
\]
\[
\Rightarrow 2d \sin \theta = n \lambda
\]
2) \( \omega(q) = 2 \sqrt{\frac{K}{m}} \sin \left( |q| \frac{a}{2} \right) \)

Note that \( \omega(q) \geq 0 \) always. There are no negative frequencies.

a) \( V_g(q) = \oint \frac{d\omega}{dq} = \alpha \sqrt{\frac{K}{m}} \cos \left( |q| \frac{a}{2} \right) \)

\( \cos \) is symmetric so we don't need the \(|q|\) but we do need the correct sign so that \( V_g(q) \) for \( q < 0 \) is negative.

\[ V_g(q) = \frac{q}{|q|} \alpha \sqrt{\frac{K}{m}} \cos \left( |q| \frac{a}{2} \right) \]

b) This is 1D so the equal energy contour is

\[ \text{---} -w = \omega, \text{ really just 2 points} \]

c) \[ D(\omega) = \frac{1}{2\pi} \cdot \frac{2}{|V_g|} = \frac{1}{|\pi V_g|} \]

\[ |V_g| = \alpha \sqrt{\frac{K}{m}} \cos \left( \frac{qa}{2} \right) \]

\[ \frac{qa}{2} = \sin^{-1} \left( \frac{\omega}{2\sqrt{\frac{m}{K}}} \right) \]

\[ |V_g| = \alpha \sqrt{\frac{K}{m}} \cos \left( \sin^{-1} \left( \frac{\omega}{2\sqrt{\frac{m}{K}}} \right) \right) \]
$$|V_g(\omega)| = a \sqrt{\frac{K}{m}} \sqrt{1 - \frac{\omega^2 m}{4K}} = a \sqrt{\frac{K}{m} - \frac{\omega^2}{4}}$$

$$D(\omega) = \frac{1}{\pi a} \sqrt{\frac{K}{m} - \frac{\omega^2}{4}}$$

Note that at $\omega = 0$, $D(\omega) = \frac{1}{\pi a} \sqrt{\frac{K}{m}}$

which matches the group velocity definition at $q = 0$ being $V_g(0) = a \sqrt{\frac{K}{m}}$

Then at $q = \frac{\pi}{a}$, $\omega = 2\sqrt{\frac{K}{m}}$ and

$$\sqrt{\frac{K}{m} - \frac{\omega^2}{4}} = 0$$

so $D(\omega)$ diverges.

e) $D(\omega)$ goes to $\infty$ at $\omega = 2\sqrt{\frac{K}{m}}$
4) \[ U_c(T_c) = \int_0^{w_0} (\text{tr}(\nu)) B(\nu) f_{NB}(\nu, T_c) \, d\nu \]

\[ = \int_0^{w_0} (\text{tr}(\nu)) \frac{\nu^2}{2\pi^2 C_s^3} e^{-\frac{\nu^2}{k_B T_c}} \, d\nu \]

\[ = \frac{(k_B T_c)^3}{2\pi^2 C_s^3 h^2} \int_0^{w_0} \left( \frac{\nu}{k_B T_c} \right)^3 e^{-\frac{\nu^2}{k_B T_c}} \, d\nu \]

Using \[ x = \frac{\nu}{k_B T_c}, \quad dx = \frac{k_B T_c}{\nu} \, d\nu \]

\[ U_c(T_c) = \left( \frac{k_B T_c}{C_s^3 h^2} \right)^4 \int_0^{\frac{k_B T_c}{C_s^3 h^2}} x^3 e^{-x} \, dx = 6 \left( \frac{k_B T_c}{C_s^3 h^2} \right)^4 \]

\[ U_a(T_a) = \int_0^{w_0} (\text{tr}(\nu)) \frac{\nu^2}{2\pi^2 C_s^3} \frac{1}{e^{\nu/k_B T_a} - 1} \, d\nu \]

After the substitution \[ x = \nu/k_B T_a \]

we get

\[ U_a(T_a) = \left( \frac{k_B T_a}{C_s^3 h^2} \right)^4 \int_0^{\frac{k_B T_a}{C_s^3 h^2}} x^3 \left( e^x - 1 \right)^{-1} \, dx \]

\[ = \frac{\zeta(4)}{5} \left( \frac{k_B T_a}{C_s^3 h^2} \right)^4 \]

\[ \text{set} \quad U_c = U_a + \quad \text{set} \quad T_c^4 = \frac{\zeta(4)}{5} T_a^4 = \frac{\pi^4}{70} \quad \text{set} \quad T_c = \frac{\pi T_a}{\zeta(4)} \]

\[ T_c = \frac{\pi T_a}{70} \]
b) In general $d$-dimensional Debye system, we would have

$$T_c^4 \int_0^\infty x^3 e^{-x} \, dx = T_0^4 \int_0^\infty x^3 (e^{-x} - 1) \, dx$$

$$T_c^4 = \frac{\pi^2}{2} \left( d+1 \right) T_0^4$$

So for a 1.-d. system, we have

$$T_c = 4\sqrt{\frac{\pi^2}{6}} T_0$$ which is a bigger difference than in 3d.
\( t_{12} = \frac{M_2}{M_1 + M_2} \)

So, a 1D system \( M_1(\omega) = 1 \)

\( M_2(\omega) \) is 2-D so \( M_2(\omega) = \frac{\omega}{2\alpha} \)

\[ t_{12} = \frac{W \omega/(2\alpha)}{1 + W \omega/(2\alpha)} = \frac{\omega}{2\alpha + \omega} \]

However, we have a units mismatch here as \( \alpha \) has units of velocity \( (m/s) \) and \( \omega \) is frequency \( (s^-1) \) so we should have added the width of the contact between the two system.

\[ t_{12}(\omega) = \frac{W \omega/(2\alpha)}{1 + W \omega/(2\alpha)} = \frac{\omega}{2 \frac{\alpha}{W} + \omega} \]

b) For a 3D system, i.e. have

\( M_3(\omega) = \frac{\omega^2}{2\pi \alpha^2} \) so

\[ t_{13}(\omega) = \frac{\omega^2/(2\pi \alpha^2)}{1 + \omega^2/(2\pi \alpha^2)} = \frac{\omega^2}{2\pi \alpha^2 + \omega^2} \]

Again, for proper dimensions, we should have \( M_3(\omega) = A \omega^2/(2\pi \alpha^2) \) to get

\[ t_{13}(\omega) = \frac{\omega^2}{2\pi \alpha^2/A + \omega^2} = \frac{A \omega^2}{2 \alpha \omega^2 + A \omega^2} \]
Indeed, if we reverse direction, we get

\[ t_{21}(\omega) = \frac{M_1(\omega)}{M_1(\omega) + M_2(\omega)} = \frac{1}{1 + \omega / (2\alpha)} \]

\[ = \frac{2\alpha}{2\alpha + \omega} \]

With proper units we have

\[ t_{21}(\omega) = \frac{2\alpha}{2\alpha + \omega} \]

and

\[ t_{31}(\omega) = \frac{1}{1 + \omega^2 / (2\pi L^2)} \]

\[ = \frac{2\pi L^2}{2\pi L^2 + \omega^2} \]

The direction from a "smaller" 1d system to a 2d or a 3d system appears to be stronger because the 1 channel of the 1d system can almost always find a channel to transmit into in the 2d or 3d system, while only 1 out of the many channels in the 2d or 3d finds a partner in the 1d system.
6. a) \[ D(\omega) = \frac{2}{\pi a \sqrt{4K/n} - \omega^2} \]

\[ = \frac{2}{\pi a \sqrt{\omega_{\text{max}}^2 - \omega^2}} \]

where \( \omega_{\text{max}} = 2\sqrt{\frac{K}{n}} \)

\[ \frac{2}{L} = \int \frac{2}{\pi a \sqrt{\omega_{\text{max}}^2 - \omega^2}} \, d\omega = \frac{2}{\pi a} \int_0^{\omega_{\text{max}}} (\omega_{\text{max}}^2 - \omega^2)^{-\frac{1}{2}} \, d\omega \]

\[ = \frac{2}{\pi a} \cdot \frac{\pi}{2} = \frac{1}{a} \]

There is no need to set an upper bound because \( \omega_{\text{max}} = 2\sqrt{\frac{K}{n}} \) which occurs at \( \omega = \pi/a \).

This is true in general in 1d, the Debye wave vector \( k_D = \pi/a \) which is already the edge of the 1d Brillouin zone.
b) \[ C(T) = \int_0^{\infty} \left( \frac{h \omega}{2} \right) D(\omega) \frac{dE}{d\omega} \frac{\hbar}{k_B} \left( \frac{\hbar \omega}{k_B T} \right) d\omega \]

\[
= \int_0^{\omega_{\text{max}}} (\hbar \omega)^2 \frac{2}{\pi a} \frac{2}{\hbar v_{\text{max}}^2 - \omega^2} \frac{e^{\frac{-\hbar \omega}{k_B T}}}{(e^{\frac{-\hbar \omega}{k_B T}} - 1)^2} \frac{d\omega}{k_B T^2}
\]

\[
= 2 \frac{k_B}{\pi a} \int_0^{\omega_{\text{max}}} \frac{(\hbar \omega)^2}{(k_B T)^2} \frac{d\omega}{\sqrt{\hbar v_{\text{max}}^2 - \omega^2}} \frac{e^{\frac{-\hbar \omega}{k_B T}}}{(e^{\frac{-\hbar \omega}{k_B T}} - 1)^2}
\]

let \( x = \frac{\hbar \omega}{k_B T} \)

\[
\omega = \frac{k_B T}{\hbar} x \quad dw = \frac{k_B T}{\hbar} dx
\]

\[
C(T) = 2 \frac{k_B}{\pi a} \int_0^{\omega_{\text{max}}/\hbar} \frac{x^2}{k_B T} \frac{dx}{\sqrt{\left(\frac{k_B T}{\hbar}\right)^2 X_{\text{max}}^2 - x^2}} \frac{e^x}{(e^x - 1)^2}
\]

\[
= 2 \frac{k_B}{\pi a} \int_0^{\omega_{\text{max}}/\hbar} \frac{x^2}{k_B T} \frac{dx}{\sqrt{1}} \frac{e^x}{(e^x - 1)^2}
\]

\[
= \frac{2 k_B}{\pi a} \int_0^{\omega_{\text{max}}/\hbar} x^2 e^x \frac{dx}{1 X_{\text{max}}^2 - X^2 (e^x - 1)^2}
\]

- See numerical part
- This function goes to \( \pi/2 \) in the high \( T \) limit
- Goes to zero linearly in the low \( T \) limit
- Transition around \( k_B T = \hbar v_{\text{max}} \)
% some predeclared values, number of points in temperature and x
Nt=2e2; Nx=2e6;
% use a logarithmic vector of temperatures to get evenly spaced points on a
% log-log plot
Tvec=logspace(-3,1,Nt);
% xmax can be written as T_D/T but we don't know what T_D is so calculate
% and plot everything in terms of the T_D/T ratio
xmax=1./Tvec;
% preallocate storage for the heat capacity vs T
CT=zeros(Nt,1);
% loop over all temperatures to get heat capacity at each T
for n=1:Nt
    % the x variable is here a vector of linearly spaced values from zero
    % to xmax with Nx points
    xvec=linspace(0,xmax(n),Nx);
    % tfun is the integrand which is dependent on x and temperature
    tfun=xvec.^2.*exp(xvec)./sqrt(xmax(n)^2-xvec.^2)./(exp(xvec)-1).^2;
    % fix the endpoints at x=0 and x=xmax so they are not Inf and NaN; the
    % actual values were found just by looking at the limits of tfun as
    % xvec goes to zero and infinity
    tfun(1)=1/xmax(n);
    tfun(Nx)=0;
    % the heat capacity is just an integral of tfun over xvec, implemented
    % here using a simple trapezoidal rule, sufficient for accuracy in 1d
    CT(n)=trapz(xvec,tfun);
end
% finally after the loop over temperatures is done, we plot the results...
loglog(2/pi*Tvec,CT)
% ...and label the plot
xlabel('T/T_D'),ylabel('C(T)/k_B')