

Q1

1.

With respect to the conventional unit cell, the reciprocal lattice vectors are of the form

$$\mathbf{K} = \frac{2\pi}{a}(h\hat{x} + k\hat{y} + l\hat{z}) \quad (1)$$

where h , k and l are integers. The geometric structure factor is then given by

$$\begin{aligned} S(\mathbf{K}) &= \sum_j e^{-i\mathbf{K}\cdot\mathbf{d}_j} = \\ &1 + e^{-i(h+k)\pi} + e^{-i(h+l)\pi} + e^{-i(k+l)\pi} + e^{-i(h+k+l)\pi/2} + \\ &e^{-i(3h+3k+l)\pi/2} + e^{-i(3h+k+3l)\pi/2} + e^{-i(h+3k+3l)\pi/2} = \\ &[1 + (-1)^{h+k} + (-1)^{k+l} + (-1)^{l+h}] [1 + (-1)^{h+k+l}] \\ &= \begin{cases} 4 \times 2, & \text{all even or all odd and } h+k+l = 4n \\ 4(1-i), & \text{all even or all odd and } h+k+l = 4n+1 \\ 4(1+i), & \text{all even or all odd and } h+k+l = 4n+3 \\ 0, & \text{otherwise} \end{cases} \quad (2) \end{aligned}$$

Note that the first factor is for the plain FCC lattice while the second factor is for the two-atom basis. The few sets of Miller indices for the reciprocal lattice vectors that give rise to nonzero geometric structure factors are listed below together with the values of the structure factor and the respective $|\mathbf{K}|$.

$[hkl]$	$S(\mathbf{K})$	$ \mathbf{K} $
[111]	$4+4i$	$\sqrt{3}\frac{2\pi}{a}$
[220]	8	$\sqrt{8}\frac{2\pi}{a}$
[311]	$4-4i$	$\sqrt{11}\frac{2\pi}{a}$
[400]	8	$4\frac{2\pi}{a}$
[331]	$4+4i$	$\sqrt{19}\frac{2\pi}{a}$

Considering the relation $|\mathbf{K}| = 2|\mathbf{k}|\sin(\phi/2)$, we deduce that the two smallest Bragg angles correspond to the smallest $|\mathbf{K}|$ which are listed in the first two rows of the table above. Hence the Miller indices of the first two diffraction angles are [111] and [220].

2.

Considering that the diffraction intensity is proportional to the absolute value squared of the geometric structure factor, we have the following intensity ratio for the first two lines

$$\frac{I_1}{I_2} = \frac{8}{12} \frac{|S([111])|^2}{|S([220])|^2} = \frac{2}{3} \frac{|4+4i|^2}{8^2} = \frac{1}{3} \quad (3)$$

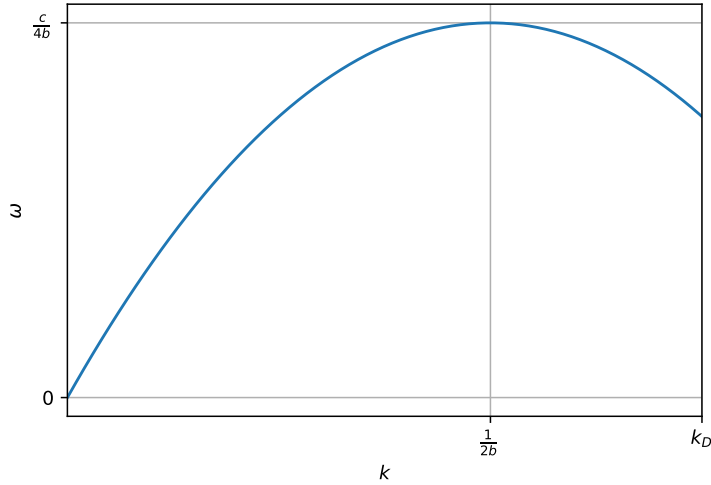
where the 8/12 factor is due to plane multiplicity.

3.

There are three significant differences caused by the described replacement. First, there would be additional diffraction lines at angles smaller than the smallest angle previously found. Specifically the diffraction angles of the underlying simple cubic lattice will not be cancelled by the geometric structure factor since it is no longer an FCC with a basis but a simple cubic with a basis. This can be seen in eq. (2) where the first 1 in the second line now has a prefactor which is different from the other terms, so that no total cancellation is possible. Second, the intensities will change, as the structure factor changes, and third, slight changes to the crystal structure will cause a broadening of the diffraction lines.

Q2

1.



$g(\omega)d\omega$ is the number of states between ω and $\omega + d\omega$. Near $\omega_m = \frac{c}{4b}$ there are two k 's for a given ω :

$$bk^2 - k + \omega/c = 0 \quad (4)$$

$$k_{\pm} = \frac{1}{2b} \left[1 \pm \sqrt{1 - 4\omega b/c} \right]$$

The density of states as a function of ω is related to the density of states as a function of k by $g(\omega)d\omega = g(k)dk$ which means

$$g(\omega) = g(k) \left| \frac{d\omega}{dk} \right|^{-1} \quad (5)$$

so for $\omega(k_D) < \omega < \omega_m$ we have

$$g(\omega) = \frac{k_-(2\pi)}{\left| \frac{d\omega}{dk} \Big|_{k_-} \right|} + \frac{k_+(2\pi)}{\left| \frac{d\omega}{dk} \Big|_{k_+} \right|}. \quad (6)$$

Using

$$\left. \frac{d\omega}{dk} \right|_{k_{\pm}} = c - 2cbk_{\pm} = \mp c\sqrt{1 - 4\omega b/c} \quad (7)$$

eq. (6) becomes

$$g(\omega) = \frac{1}{2\pi c\sqrt{1 - 4\omega b/c}} \left[1 + \sqrt{1 - 4\omega b/c} + 1 - \sqrt{1 - 4\omega b/c} \right] \frac{1}{2b} = \frac{1}{2\pi bc\sqrt{1 - \omega/\omega_m}} \quad (8)$$

For $\omega < \omega(k_D)$ only k_- is relevant so

$$g(\omega) = \frac{1 - \sqrt{1 - 4\omega b/c}}{4\pi bc\sqrt{1 - 4\omega b/c}} = \frac{1 - \sqrt{1 - \omega/\omega_m}}{4\pi bc\sqrt{1 - \omega/\omega_m}} \quad (9)$$

2.

We have already found $\omega_m = \frac{c}{4b}$ and looking at eq. (8) one sees that the singularity has $\gamma = \frac{1}{2}$.

3.

For $k_B T \ll \hbar\omega(k_D)$ we take the dispersion relation to be linear, $\omega = ck$, so that the total energy is

$$\frac{E}{A} = \int \frac{d^2k}{(2\pi)^2} \frac{\hbar\omega(k)}{e^{\beta\hbar\omega(k)} - 1} = \int \frac{kdk}{2\pi} \frac{\hbar ck}{e^{\beta\hbar ck} - 1} = \frac{\hbar c}{2\pi} \left(\frac{k_B T}{\hbar c} \right)^3 \int_0^\infty \frac{x^2 dx}{e^x - 1} \quad (10)$$

where we performed the change of variables $x = \beta\hbar ck$ and took the upper limit to ∞ where the integrand is exponentially small. The heat capacity is then,

$$c_V = \frac{3k_B^3 T^2}{2\pi\hbar^2 c^2} \int_0^\infty \frac{x^2 dx}{e^x - 1} \sim T^2 \quad (11)$$

4.

For $k_B T \gg \hbar\omega(k_D)$ we expand the exponent in the denominator in eq. (10) to $e^{\beta\hbar\omega} \simeq 1 + \beta\hbar\omega$ so that

$$\frac{E}{A} = k_B T \int \frac{d^2k}{(2\pi)^2} = \frac{k_B T}{a^2} \quad (12)$$

and

$$c_V = k_B/a^2 \quad (13)$$

Q3

1.

For a one-dimensional lattice, the electron wave function in the Bloch form is

$$\phi_k(r) = \frac{1}{\sqrt{N}} \sum_l e^{ikR_l} \psi(r - R_l) \quad (14)$$

where N is the number of atoms in the lattice. Then the energy of the electron is

$$\epsilon_k = \langle \phi_k | H | \phi_k \rangle = \frac{1}{N} \sum_{l, l'} e^{ik(R_l - R_{l'})} \langle \psi(r - R_l) | H | \psi(r - R_{l'}) \rangle. \quad (15)$$

As only nearest-neighbor interactions are nonzero, we have

$$\begin{aligned} \epsilon_k &= \frac{1}{N} \sum_l \left[\langle \psi(r - R_l) | H | \psi(r - R_l) \rangle \right. \\ &\quad + e^{-ikb} \langle \psi(r - R_l) | H | \psi(r - R_{l+1}) \rangle \\ &\quad \left. + e^{ikb} \langle \psi(r - R_l) | H | \psi(r - R_{l-1}) \rangle \right] \\ &= -E_0 - V (e^{-ikb} + e^{ikb}) \\ &= -E_0 - 2V \cos(kb) \end{aligned} \quad (16)$$

2.

In 1D the density of states per unit length for electrons is given by

$$g(k) = \frac{2}{L} \frac{dN}{dk} = \frac{2}{L} \frac{d}{dk} \left(\frac{kL}{\pi} \right) = \frac{2}{\pi} \quad (17)$$

where the factor of 2 is due to the 2 spin states. As a function of energy it is

$$\begin{aligned} g(\epsilon) &= g(k) \left(\frac{d\epsilon}{dk} \right)^{-1} = \frac{1}{\pi V b \sin(kb)} \\ &= \frac{1}{\pi b V \sqrt{1 - \left(\frac{\epsilon + E_0}{2V} \right)^2}} \end{aligned} \quad (18)$$

3.

At $T = 0$ the energy of the electrons is

$$E = L \int_0^{k_F} \epsilon_k g(k) dk \quad (19)$$

where k_F is determined by

$$N = L \int_0^{k_F} g(k) dk = \frac{2L}{\pi} k_F \implies k_F = \frac{\pi n}{2b} \quad (20)$$

where n is the number of electrons per unit cell. So solving eq. (19),

$$\begin{aligned} E &= L \int_0^{\frac{\pi n}{2b}} (-E_0 - 2V \cos(kb)) \frac{2}{\pi} dk = \frac{2Nb}{\pi} \left(-E_0 k - \frac{2V}{b} \sin(kb) \right) \Big|_0^{\frac{\pi n}{2b}} = \\ &\quad -E_0 N - \frac{4NV}{\pi} \sin\left(\frac{\pi n}{2}\right) \end{aligned} \quad (21)$$

In this section $n = 1$ so each electron on average contributes $-\frac{4V}{\pi}$ relative to $-E_0$ to the total energy.

4.

In this section $n = 2$ so each electron on average contributes 0 relative to $-E_0$ to the total energy. In this case $k_F = \frac{\pi}{b}$ so the electrons occupy all of the states within the only energy band. In this configuration the system is not a conductor.