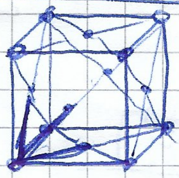
Disclaimer

The solution at hand was written in the course of the respective class at the University of Bonn. If not stated differently on top of the first page or the following website, the solution was prepared and handed in solely by me, Marvin Zanke. Anything in a different color than the ball pen blue is usually a correction that I or a tutor made. For more information and all my material, check:
https://www.physics-and-stuff.com/

I raise no claim to correctness and completeness of the given solutions! This equally applies to the corrections mentioned above.

04.05.'16 Condensed Matter Exercise 2

1 a) fcc



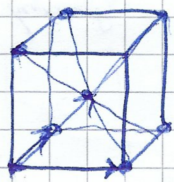
$l = \frac{a}{\sqrt{2}}$

$\Rightarrow a_1 = \frac{a}{2}(\vec{e}_x + \vec{e}_y)$, $a_3 = \frac{a}{2}(\vec{e}_x + \vec{e}_z)$

$a_2 = \frac{a}{2}(\vec{e}_y + \vec{e}_z)$

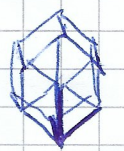
"Space lattice"?

bcc



$a_1 = a\vec{e}_x$, $a_2 = a\vec{e}_y$, $a_3 = \frac{a}{2}(\vec{e}_x + \vec{e}_y + \vec{e}_z)$

hexagonal



$a_1 = \frac{\sqrt{3}}{2} a\vec{e}_x + \frac{1}{2} a\vec{e}_y$,

$a_2 = a\vec{e}_y$, $a_3 = c\vec{e}_z$

always primitive translation vectors as unit cell? Yes

b)

fcc: $\overset{\begin{pmatrix}1\\0\\1\end{pmatrix}}{\left[\frac{a}{2}(\vec{e}_x + \vec{e}_z)\right]} \cdot \left\{ \underbrace{\overset{\begin{pmatrix}0\\1\\1\end{pmatrix}}{\left[\frac{a}{2}(\vec{e}_y + \vec{e}_z)\right]} \times \overset{\begin{pmatrix}1\\1\\0\end{pmatrix}}{\left[\frac{a}{2}(\vec{e}_x + \vec{e}_y)\right]}}_{\frac{a^2}{4}\left\{(-\vec{e}_z) + \vec{e}_y - \vec{e}_x\right\} = \frac{a^2}{4}\begin{pmatrix}-1\\1\\-1\end{pmatrix}} \right\}$

$= \frac{a^3}{8}(-1-1) \Rightarrow V_u = \frac{a^3}{4}$

bcc: $\left[\frac{a}{2}(\vec{e}_x + \vec{e}_y + \vec{e}_z)\right] \cdot \left\{ \underbrace{[a\vec{e}_x] \times [a\vec{e}_y]}_{a^2\vec{e}_z} \right\}$

$= \frac{a^3}{2}$

hexagonal: $\left[\frac{\sqrt{3}}{2} a\vec{e}_x + \frac{1}{2} a\vec{e}_y\right] \cdot \left\{ \underbrace{(a\vec{e}_y) \times (c\vec{e}_z)}_{ac\vec{e}_x} \right\}$

$= \frac{\sqrt{3}\, a^2 c}{2}$

Aufgabe 4: 1-dim rechnen

c) fcc: $b_1 = 2\pi \frac{a_2 \times a_3}{a_1 \cdot (a_2 \times a_3)} = 2\pi \frac{\frac{a^2}{4}\begin{pmatrix}1\\1\\-1\end{pmatrix}}{\frac{a^3}{4}} = \frac{2\pi}{a}\begin{pmatrix}1\\1\\-1\end{pmatrix}$

$b_3 = 2\pi \frac{a_1 \times a_2}{V} = 2\pi \frac{\frac{a^2}{4}\begin{pmatrix}+1\\-1\\+1\end{pmatrix}}{a^3/4} = \frac{2\pi}{a}\begin{pmatrix}+1\\-1\\+1\end{pmatrix}$

See this faster?

$b_2 = 2\pi \frac{a_3 \times a_1}{V} = \frac{2\pi}{a}\begin{pmatrix}-1\\1\\1\end{pmatrix}$

Symmetry reasons

$b_1 = \begin{pmatrix}-2\pi/a\\-2\pi/a\\0\end{pmatrix}$ $b_2 = \begin{pmatrix}-2\pi/a\\0\\-2\pi/a\end{pmatrix}$ $b_3 = \begin{pmatrix}0\\-2\pi/a\\-2\pi/a\end{pmatrix}$

bcc: $b_1 = 2\pi \frac{\begin{pmatrix}1\\0\\-1\end{pmatrix}\frac{a^2}{2}}{a^3/2} = \frac{2\pi}{a}\begin{pmatrix}1\\0\\-1\end{pmatrix}$

$b_2 = 2\pi \frac{\begin{pmatrix}0\\1\\-1\end{pmatrix}\frac{a^2}{2}}{a^3/2} = \frac{2\pi}{a}\begin{pmatrix}0\\1\\-1\end{pmatrix}$

$b_3 = 2\pi \frac{\begin{pmatrix}0\\0\\1\end{pmatrix}a^2}{a^3/2} = \frac{4\pi}{a}\begin{pmatrix}0\\0\\1\end{pmatrix}$

hexagonal: $b_1 = 2\pi \frac{ac\begin{pmatrix}1\\0\\0\end{pmatrix}}{\frac{\sqrt{3}a^2c}{2}} = \frac{4\pi}{a\sqrt{3}}\begin{pmatrix}1\\0\\0\end{pmatrix}$

$b_1 = \begin{pmatrix}2\pi/\sqrt{3}a\\2\pi/a\\0\end{pmatrix}$

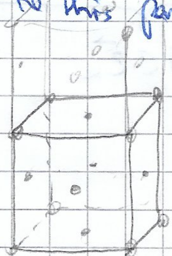
$b_2 = 2\pi \frac{\begin{pmatrix}-ac/2\\\frac{\sqrt{3}}{2}ac\\0\end{pmatrix}2}{\sqrt{3}a^2c} = \frac{4\pi}{2\sqrt{3}a}\begin{pmatrix}-1\\\sqrt{3}\\0\end{pmatrix} = \frac{2\pi}{\sqrt{3}a}\begin{pmatrix}-1\\\sqrt{3}\\0\end{pmatrix}$

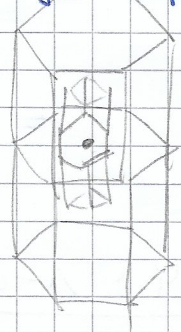
$b_3 = 2\pi \frac{\begin{pmatrix}0\\0\\\frac{\sqrt{3}}{2}a^2\end{pmatrix}2}{\sqrt{3}a^2c} = \frac{2\pi}{c}\begin{pmatrix}0\\0\\1\end{pmatrix}$

Anschaulich?

d) Distance to all points / lattice vectors in the reciprocal lattice is the same for the first Brillouin Zone and it contains 1 lattice point. Distance to this point is smaller than distance to any other point.

fcc





Wigner Seitz-Cell in reciprocal lattice

2 a) - We have a bcc lattice, where each Cs-Ion counts $\frac{1}{8}$ to the number of atoms, in a unit cell. The Jodine ion counts 1 each in our unit cell.

Is form factor really for one single atom?

yes, x-ray because cross-section large only for electrons

- $\rightarrow \rho_j(r')$ is (about) the same for both ions in the CsI Crystal
- the Volume (we integrate over) is almost the same for both atoms, as they both have ~54 electrons and almost the same nuclei.
- $f_j(G) = \int_{V_j} \rho_j(r') e^{-iGr'} dV'$
- x-ray diffraction because of the high energy ($\rightarrow$ Small wavelength) and thereby
- atomic number 56 / 54 $\xrightarrow{ion}$ same number electrons (most important)

b) $S_G = \sum_j f_j(G) e^{-2\pi i(hu_j + kv_j + lw_j)}$

Why can it be?

Have to be integers?

For which diffraction peaks?

bcc lattice can be regarded as a sc lattice, with a unit cell containing 2 atoms located at $r_1 = 0$, $r_2 = \frac{a}{2}(\vec{e_x} + \vec{e_y} + \vec{e_z})$

$$S_G \overset{a)}{=} f(G) \{ e^{-2\pi i(0h + 0k + 0l)} + e^{-\pi i(h+k+l)} \}$$

$$= f(G) \{ 1 + e^{-\pi i(h+k+l)} \} = \begin{cases} 2f(G), & h+k+l \text{ even} \\ 0, & h+k+l \text{ odd} \end{cases}$$

3

$$U(T) = \int_0^{\omega_E} D(\omega)\, E(\omega, T)\, d\omega = 3N \int_0^{\omega_E} \delta(\omega - \omega_E)\, E(\omega, T)\, d\omega$$

$$= 3N\, E(\omega_E, T) = 3N \left\{ \hbar\omega_E \left(\frac{1}{2} + \frac{1}{e^{\hbar\omega_E/k_BT} - 1} \right) \right\}$$

$$\Rightarrow \frac{\partial U}{\partial T} = C_V = 3N\hbar\omega_E \frac{-1}{\left(e^{\hbar\omega_E/k_BT} - 1\right)^2} \cdot e^{\hbar\omega_E/k_BT} \left(-\frac{\hbar\omega_E}{k_B T^2} \right)$$

$$= \frac{3N\hbar^2\omega_E^2}{k_B T^2} \frac{e^{\hbar\omega_E/k_BT}}{\left(e^{\hbar\omega_E/k_BT} - 1\right)^2}$$

$$= 3Nk_B \left(\frac{\theta_E}{T}\right)^2 \frac{e^{\theta_E/T}}{\left(e^{\theta_E/T} - 1\right)^2}$$

$$\overset{T \gg \theta_E}{=} 3Nk_B$$

$$\overset{T \ll \theta_E}{=} 3Nk_B \left(\frac{\theta_E}{T}\right)^2 e^{-\theta_E/T}$$

$E(\omega T)$ always the same because phonons are bosons

Follow Bose-Einstein distribution because they have Spin = 1.

$(2\pi)^2$ or $\frac{(2\pi)^3}{(2\pi)^2}$

4 $\frac{\partial\omega}{\partial k} = c$ with $\omega = ck$ dispersion relation

$$\Rightarrow D(\omega) = \frac{V_c}{(2\pi)^2}\int_{C(\omega)} \frac{dC_\omega}{c} = \frac{V_c}{(2\pi)^2 c}\, 2\pi k(\omega)$$

$$= \frac{V_c}{2\pi c}\, k(\omega) = \frac{V_c}{2\pi c^2}\,\omega$$

$V_c \mapsto A_c$

$D = D_L + D_T = \frac{A_c}{\pi}\frac{\omega}{c_D^2}$

N(ω) not needed

not needed

$$N(\omega) = \int_0^\omega D(\omega')\,d\omega' = \frac{V_c}{2\pi c^2}\frac{1}{2}\omega^2$$

$\frac{1}{c_L^2} + \frac{1}{c_T^2} = \frac{2}{c_D^2}$

$$\Leftrightarrow \frac{N_c}{V_c} 2\pi c^2 \boxed{2} = \omega^2 \Leftrightarrow \sqrt{\frac{2\,4\pi c^2 N_c}{V_c}} = \omega$$

this does not contribute to $C_V(T)$

$$U(T) = \int_0^{\omega_D} D(\omega)\,E(\omega,T)\,d\omega = \frac{V_c}{\boxed{2}\pi c^2}\int_0^{\omega_D} \hbar\omega^2\left(\frac{1}{2} + \frac{1}{e^{\hbar\omega/k_BT}-1}\right)d\omega$$

$$\Rightarrow U'(T) = \frac{V_c\hbar}{\boxed{2}\pi c^2}\int_0^{\omega_D}\frac{\omega^2}{e^{\hbar\omega/k_BT}-1}\,d\omega$$

atoms are cooled down to graphite surface $\Rightarrow T \ll \frac{\hbar\omega}{k_B}$

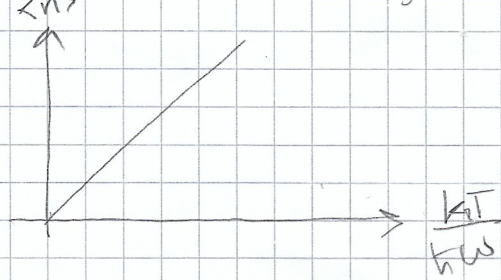
$$= \frac{V_c\hbar}{\boxed{2}\pi c^2}\int_0^\infty \omega^2 e^{-\frac{\hbar\omega}{k_BT}}\,d\omega$$

$$= \frac{V_c\hbar}{\boxed{2}\pi c^2}\frac{2k_B^3T^3}{\hbar^3} = \frac{V_c k_B^3 T^3}{\pi\hbar^2 c^2}\,2$$

$$\Rightarrow C_V = \left(\frac{\partial U}{\partial T}\right)_V = \frac{6V_c k_B^3 T^2}{\hbar^2 c^2 \pi} \propto T^2$$

5

$$\langle n\rangle = \frac{1}{e^{\hbar\omega/k_BT}-1} = \begin{cases} e^{-\hbar\omega/k_BT} & \text{for small } T \\ \frac{1}{1+\frac{\hbar\omega}{k_BT}-1} = \frac{k_BT}{\hbar\omega} & \text{for large } T\end{cases}$$



Debye approx:

$$\langle n \rangle = \int_0^{\omega_D} D(\omega) \langle n(\omega) \rangle \, d\omega$$

$$D(\omega) = \frac{3V_c}{2\pi^2} \frac{\omega^2}{c_D^3}$$

$$x = \frac{\hbar\omega}{k_B T}, \quad dx = \frac{\hbar}{k_B T} d\omega, \quad x_D = \frac{\hbar\omega_D}{k_B T} = \frac{\theta_D}{T}$$

$$\langle n \rangle = \frac{3V_c}{2\pi^2 c_D^3} \left(\frac{k_B T}{\hbar} \right)^3 \underbrace{\int_0^{x_D} \frac{x^2}{e^x - 1}}_{T \ll 1: \left(\frac{\theta_D}{T}\right)} dx$$

$T \gg \theta_D$: $x \ll 1$

$T \ll \theta_D$: $x_D \to \infty$

$$\langle n \rangle = \begin{cases} T^3 & T \ll \theta \\ T & T \gg \theta \end{cases}$$