Mid term test of Condensed Matter Physics - November 25th 2022
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Exercise 1: Bravais lattices and X-ray scattering.

Consider a monoatomic compound A that forms orthorhombic crystals. The sides of the primitive cell are $a = 0.2\,\text{nm}$, $b = 2a = 0.4\,\text{nm}$, and $c = 3a = 0.6\,\text{nm}$. The vectors $\boldsymbol{a}_1 = a\,\hat{\boldsymbol{x}}$, $\boldsymbol{a}_2 = b\,\hat{\boldsymbol{y}} = 2a\,\hat{\boldsymbol{y}}$, and $\boldsymbol{a}_3 = c\,\hat{\boldsymbol{z}} = 3a\,\hat{\boldsymbol{z}}$ are adopted as primitive vectors, $\hat{\boldsymbol{x}}$, $\hat{\boldsymbol{y}}$, and $\hat{\boldsymbol{z}}$ being the unit vectors of the corresponding axes.

1. [4 points] Determine the expressions of the primitive vectors of the reciprocal lattice $\boldsymbol{b}_1$, $\boldsymbol{b}_2$, $\boldsymbol{b}_3$, and of a generic reciprocal lattice vector $\boldsymbol{K} = h\,\boldsymbol{b}_1 + k\,\boldsymbol{b}_2 + \ell\,\boldsymbol{b}_3$.

2. [7 points] Determine the numerical values of scattering angles $\varphi = 2\vartheta$ (in degrees, $^\circ$) of the first six peaks (in ascending order) that are observed if the structure of the given crystal is investigated by means of the Debye-Scherrer technique, with a radiation of wavelength $\lambda = \frac{a}{2} = 0.1\,\text{nm}$. Associate each peak to the indices $(hk\ell)$ identifying the families of lattice planes that produce it.

3. [4 points] Suppose now that a homonuclear molecule A_2 forms crystals with the same structure as A, with the two atoms located at the basis points $\boldsymbol{d}_1 = \boldsymbol{0}$ (the null vector) and $\boldsymbol{d}_2 = \frac{1}{2}\,(a\,\hat{\boldsymbol{x}} + b\,\hat{\boldsymbol{y}} + c\,\hat{\boldsymbol{z}}) = \frac{a}{2}\,(\hat{\boldsymbol{x}} + 2\hat{\boldsymbol{y}} + 3\hat{\boldsymbol{z}})$, respectively. Determine which of the six peaks found above would now be missing due to the destructive interference of the X rays scattered by the two identical atoms. Explain why the sixth peak is weakened but does not disappear.

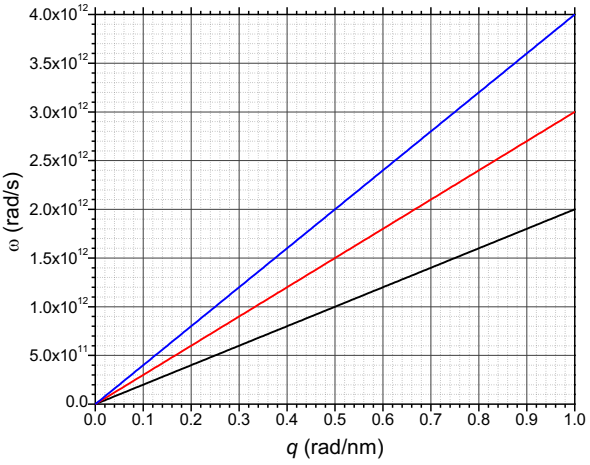

Fig. 1.

Exercise 2: Phonons and specific heat.

Consider a monoatomic cubic lattice, whose phonon dispersion curves along the $\Gamma-$M $[(0,0,0)-(\frac{\pi}{a},\frac{\pi}{a},0)]$ direction of the first Brillouin zone are displayed in Fig. 1 (notice that this is a detail in the low-q limit, the horizontal axis does not reach the boundary of the Brillouin zone). Assume that the linear dispersion relationships are valid at all wave vectors q, with sound velocities independent of the direction (Debye approximation).

1. [5 points] Evaluate the Debye frequency ω_D, knowing that the density of states at that frequency is $g(\omega = \omega_\text{D}) = 1.20 \times 10^{15}\,(\text{rad/s})^{-1}\text{m}^{-3}$ (take for the sound velocity the properly averaged value $\overline{v}$).

2. [2 points] Evaluate the atomic density n.

3. [5 points] Evaluate the specific heat c_V at the temperatures $T = 1\,\text{K}$ and $T = 500\,\text{K}$.

4. [3 points] If the lattice had a three-atom basis how the values of the specific heat at the two temperatures considered above would have been changed? Motivate your answer, under the assumption that the characteristic frequencies of the optical modes are of the same order of magnitude as ω_D.

[Useful constants: the Planck constant is $\hbar = 1.05\times10^{-34}\,\text{J·s/rad}$, the Boltzmann constant is $\kappa_\text{B} = 1.38\times10^{-23}\,\text{J·K}^{-1}$].

Solution
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Exercise 1.

1. One has

$$\boldsymbol{b}_1 = \frac{2\pi\,(\boldsymbol{a}_2 \times \boldsymbol{a}_3)}{\boldsymbol{a}_1 \cdot (\boldsymbol{a}_2 \times \boldsymbol{a}_3)} = \frac{2\pi}{a}\hat{\boldsymbol{x}}, \qquad \boldsymbol{b}_2 = \frac{2\pi\,(\boldsymbol{a}_3 \times \boldsymbol{a}_1)}{\boldsymbol{a}_1 \cdot (\boldsymbol{a}_2 \times \boldsymbol{a}_3)} = \frac{2\pi}{b}\hat{\boldsymbol{y}} = \frac{\pi}{a}\hat{\boldsymbol{y}}, \qquad \boldsymbol{b}_3 = \frac{2\pi\,(\boldsymbol{a}_1 \times \boldsymbol{a}_2)}{\boldsymbol{a}_1 \cdot (\boldsymbol{a}_2 \times \boldsymbol{a}_3)} = \frac{2\pi}{c}\hat{\boldsymbol{z}} = \frac{2\pi}{3a}\hat{\boldsymbol{z}},$$

hence $\boldsymbol{K} = h\,\boldsymbol{b}_1 + k\,\boldsymbol{b}_2 + \ell\,\boldsymbol{b}_3 = \frac{\pi}{3a}\,(6h\,\hat{\boldsymbol{x}} + 3k\,\hat{\boldsymbol{y}} + 2\ell\,\hat{\boldsymbol{z}})$.

2. The magnitude of a generic reciprocal lattice vector is $K = |\boldsymbol{K}| = \frac{\pi}{3a}\sqrt{36\,h^2 + 9\,k^2 + 4\,\ell^2}$, hence, from the Debye-Scherrer formula

$$\sin\frac{\varphi}{2} = \frac{\lambda K}{4\pi} \qquad \Rightarrow \qquad \varphi = 2\arcsin\frac{\lambda K}{4\pi},$$

with

$$\frac{\lambda K}{4\pi} = \frac{1}{24}\sqrt{36\,h^2 + 9\,k^2 + 4\,\ell^2}.$$

The first six peaks are: $\varphi_1 = 2\arcsin\frac{1}{12} = 9.56°$, corresponding to the family of lattice planes (001); $\varphi_2 = 2\arcsin\frac{1}{8} = 14.36°$, corresponding to the family of lattice planes (010); $\varphi_3 = 2\arcsin\frac{\sqrt{13}}{24} = 17.28°$, corresponding to the family of lattice planes (011); $\varphi_4 = 2\arcsin\frac{1}{6} = 19.19°$, corresponding to the family of lattice planes (002); $\varphi_5 = 2\arcsin\frac{5}{24} = 24.05°$, corresponding to the family of lattice planes (012); $\varphi_6 = 2\arcsin\frac{1}{4} = 28.96°$, corresponding to the families of lattice planes (100), (020), and (003).

3. The structure factor, if the two atoms occupying the basis points are identical, is

$$\mathcal{S}_{\boldsymbol{K}} = \sum_{j=1,2} \mathrm{e}^{\mathrm{i}\boldsymbol{K}\cdot\boldsymbol{d}_j} = 1 + \mathrm{e}^{\mathrm{i}\pi(h+k+\ell)}.$$

Therefore, the peaks that are suppressed by the destructive interference from the basis are those such that $h + k + \ell$ is an odd number. This is the case for φ_1, φ_2, and φ_5. Instead, the peak observed at the angle φ_6 is only attenuated, because the contribution from the family of lattice planes (020) survives. This is possible because the three families of lattice planes (100), (020), and (003) are not connected by the symmetries of the orthorhombic lattice. The fact that they contribute to the same peak is a consequence of the very peculiar structure of the given lattice, with $b = 2a$ and $c = 3a$, and one can be easily convinced that the three families would give rise to three different peaks if $b \neq 2a$ and $c \neq 3a$.

Exercise 2.

NOTICE that in this exercise the density of states was meant to be that of an individual acoustic branch. However, since this statement was inadvertently omitted, solutions in which the density of states is assumed to be the cumulative one (i.e., the one summed over the three acoustic branches) will also be considered as correct. The two solutions are discussed hereafter.

1. From the plot it can be found that the sound velocities for each phonon branch are $v_1 = 2000\,\mathrm{m/s}$, $v_2 = 3000\,\mathrm{m/s}$, and $v_3 = 4000\,\mathrm{m/s}$. This results in an average sound velocity given by

$$\overline{v} = \frac{1}{\sqrt[3]{\frac{1}{3}\left(\frac{1}{v_1^3} + \frac{1}{v_2^3} + \frac{1}{v_3^3}\right)}} = 2565.52\,\mathrm{m/s}.$$

Since the density of states of an individual acoustic branch, in the Debye approximation, is

$$g(\omega) = \frac{\omega^2}{2\pi^2\overline{v}^3},$$

putting $\omega = \omega_\mathrm{D}$, we find

$$\omega_\mathrm{D} = \sqrt{2\pi^2\overline{v}^3 g(\omega_\mathrm{D})} = 2.0 \times 10^{13}\,\mathrm{rad/s}.$$

2. The atomic density can be equivalently found as

$$n = \int_0^{\omega_\mathrm{D}} \frac{\omega^2}{2\pi^2\overline{v}^3}\mathrm{d}\omega = \frac{\omega_\mathrm{D}^3}{6\pi^2\overline{v}^3} = 8.0 \times 10^{27}\,\mathrm{m}^{-3},$$

or using $n = q_\mathrm{D}^3/(6\pi^2)$, with $q_\mathrm{D} = \omega_\mathrm{D}/\overline{v}$.

3. Since the Debye temperature is $\Theta_\mathrm{D} = \hbar\omega_\mathrm{D}/\kappa_\mathrm{B} = 153\,\mathrm{K}$, at $T = 1\,\mathrm{K}$ the system is in the low-temperature limit and

$$c_V = 234\left(\frac{T}{\Theta_\mathrm{D}}\right)^3 n\kappa_\mathrm{B} = 7.22\,\mathrm{J/(K\cdot m^3)}.$$

At $T = 500\,\mathrm{K}$ (much higher than Θ_D), $c_V = 3n\kappa_\mathrm{B} = 3.31 \times 10^5\,\mathrm{J/(K{\cdot}m^3)}$.

4. In the case of a three-atom basis, the specific heat at $T = 1\,\mathrm{K}$ is the same, since no optical phonon would be most likely excited. For $T = 500\,\mathrm{K}$, instead, the system is likely in the high-temperature (Dulong-Petit) regime and $c_V = 9n\kappa_\mathrm{B} = 9.94 \times 10^5\,\mathrm{J/(K{\cdot}m^3)}$.

ALTERNATIVE SOLUTION:

1a. From the plot it can be found that the sound velocities for each phonon branch are $v_1 = 2000\,\mathrm{m/s}$, $v_2 = 3000\,\mathrm{m/s}$, and $v_3 = 4000\,\mathrm{m/s}$. This results in an average sound velocity given by

$$\overline{v} = \frac{1}{\sqrt[3]{\frac{1}{3}\left(\frac{1}{v_1^3} + \frac{1}{v_2^3} + \frac{1}{v_3^3}\right)}} = 2565.52\,\mathrm{m/s}.$$

Since the cumulative density of states in the Debye approximation is

$$g(\omega) = \frac{3\omega^2}{2\pi^2\overline{v}^3},$$

putting $\omega = \omega_\mathrm{D}$, we find

$$\omega_\mathrm{D} = \sqrt{\frac{2\pi^2\overline{v}^3 g(\omega_\mathrm{D})}{3}} = 1.15 \times 10^{13}\,\mathrm{rad/s}.$$

2a. The atomic density can be equivalently found as

$$n = \frac{1}{3}\int_0^{\omega_\mathrm{D}} \frac{3\omega^2}{2\pi^2\overline{v}^3}\mathrm{d}\omega = \frac{\omega_\mathrm{D}^3}{6\pi^2\overline{v}^3} = 1.54\times10^{27}\,\mathrm{m}^{-3},$$

or using $n = q_\mathrm{D}^3/(6\pi^2)$, with $q_\mathrm{D} = \omega_\mathrm{D}/\overline{v}$.

3a. Since the Debye temperature is $\Theta_\mathrm{D} = \hbar\omega_\mathrm{D}/\kappa_\mathrm{B} = 88.3\,\mathrm{K}$, at $T = 1\,\mathrm{K}$ the system is in the low-temperature limit and

$$c_V = 234\left(\frac{T}{\Theta_\mathrm{D}}\right)^3 n\kappa_\mathrm{B} = 7.22\,\mathrm{J}/(\mathrm{K}\cdot\mathrm{m}^3).$$

At $T = 500\,\mathrm{K}$ (much higher than Θ_D), $c_V = 3n\kappa_\mathrm{B} = 6.37\times10^4\,\mathrm{J}/(\mathrm{K}\cdot\mathrm{m}^3)$.

4a. In the case of a three-atom basis, the specific heat at $T = 1\,\mathrm{K}$ is the same, since no optical phonon would be most likely excited. For $T = 500\,\mathrm{K}$, instead, the system is likely in the high-temperature (Dulong-Petit) regime and $c_V = 9n\kappa_\mathrm{B} = 1.91\times10^5\,\mathrm{J}/(\mathrm{K}\cdot\mathrm{m}^3)$.