UNOFFICIAL SOLUTIONS BY TheLongCat

C3: CONDENSED MATTER PHYSICS

TRINITY TERM 2019

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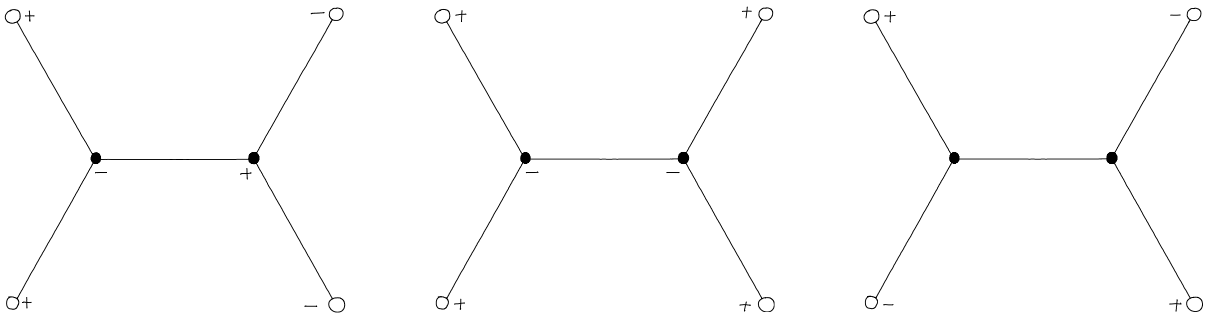
Disclaimer: due to its unofficial nature, the author does not warrant the accuracy of the presented solutions in any form. However, the author is happy to discuss the typos and errors should one arises.

Turn over as you please – we are NOT under exam conditions here.

1. (DRAFT) Symmetry and active modes.

(a) i. IR spectroscopy involves shining an infrared beam through a sample and measuring the absorption. The absorption corresponds to the energy taken to excite a vibrational mode via the electric dipole interaction. Since the electric dipole is involved, the mode must possess similar symmetry to a component of polarisation.



ii. For V_1:

$$m_x : -1 \qquad m_y : +1 \qquad m_z : -1$$

For V_2:

$$m_x : +1 \qquad m_y : +1 \qquad m_z : -1$$

For V_3:

$$m_x : -1 \qquad m_y : -1 \qquad m_z : -1$$

Character table for polarisation:

	m_x	m_y	m_z
p_x	-1	$+1$	$+1$
p_y	$+1$	-1	$+1$
p_z	$+1$	$+1$	-1

So only V_2 is IR active in p_z.

iii.

$$\begin{aligned} \#\text{ of modes} &= 3 \times 6 \quad \text{atoms} \\ &= 18 \\ &= \underbrace{\#\text{ translational}}_{3} + \underbrace{\#\text{ rotational}}_{3} + \#\text{ vibrational} \end{aligned}$$

So we have 9 additional vibration modes.

(b) # of phonon modes: # of particles in a primitive UC $= 4$

There are 2 acoustic modes and 2 optic modes.

(c) i. From the diagram,

$$\begin{aligned}
\mathbf{a}_r &= \mathbf{a}_p + \mathbf{b}_p \\
\mathbf{b}_r &= \mathbf{b}_p - \mathbf{a}_p \\
\Rightarrow \mathbf{b}_p &= \frac{\mathbf{a}_r + \mathbf{b}_r}{2} \\
\mathbf{a}_p &= \frac{\mathbf{a}_r - \mathbf{b}_r}{2}
\end{aligned}$$

ii. Definition of reciprocal basis:

$$\mathbf{a}_p^* = 2\pi \frac{\mathbf{b}_p \times \mathbf{z}}{\mathbf{a}_p \cdot (\mathbf{b}_p \times \mathbf{z})}$$

$$\begin{aligned}
\Rightarrow \mathbf{a}_p^* &= 2\pi \cdot \frac{1}{V} \cdot \frac{1}{2} \left(\underbrace{\mathbf{a}_r \times \mathbf{z}}_{-\mathbf{b}_r^* \cdot 2V/2\pi} + \underbrace{\mathbf{b}_r \times \mathbf{z}}_{\mathbf{a}_r^* \cdot 2V/2\pi} \right) \quad \text{since rectangular lattice has } 2\times\text{area} \\
&= (\mathbf{a}_r^* - \mathbf{b}_r^*) \\
\mathbf{b}_p^* &= \frac{2\pi}{V} \cdot \frac{1}{2} \left(\underbrace{\mathbf{z} \times \mathbf{a}_r}_{\mathbf{b}_r^* \cdot 2V/2\pi} - \underbrace{\mathbf{z} \times \mathbf{b}_r}_{-\mathbf{a}_r^* \cdot 2V/2\pi} \right) \\
&= \mathbf{a}_r * + \mathbf{b}_r^*
\end{aligned}$$

So Miller indices

$$\begin{array}{rr}
 & h_p\mathbf{a}_p^* = h_p\mathbf{a}_r^* - h_p\mathbf{b}_r^* \\
+) & k_p\mathbf{b}_p^* = k_p\mathbf{a}_r^* + k_p\mathbf{b}_r^* \\
\hline
 & h_p\mathbf{a}_p^* + k_p\mathbf{b}_p^* = \underbrace{(h_p + k_p)}_{h_r} \mathbf{a}_r^* + \underbrace{(-h_p + k_p)}_{k_r} \mathbf{b}_r^*
\end{array}$$

$$\Rightarrow k_p = \frac{h_r + k_r}{2} \qquad h_p = \frac{h_r - k_r}{2}$$

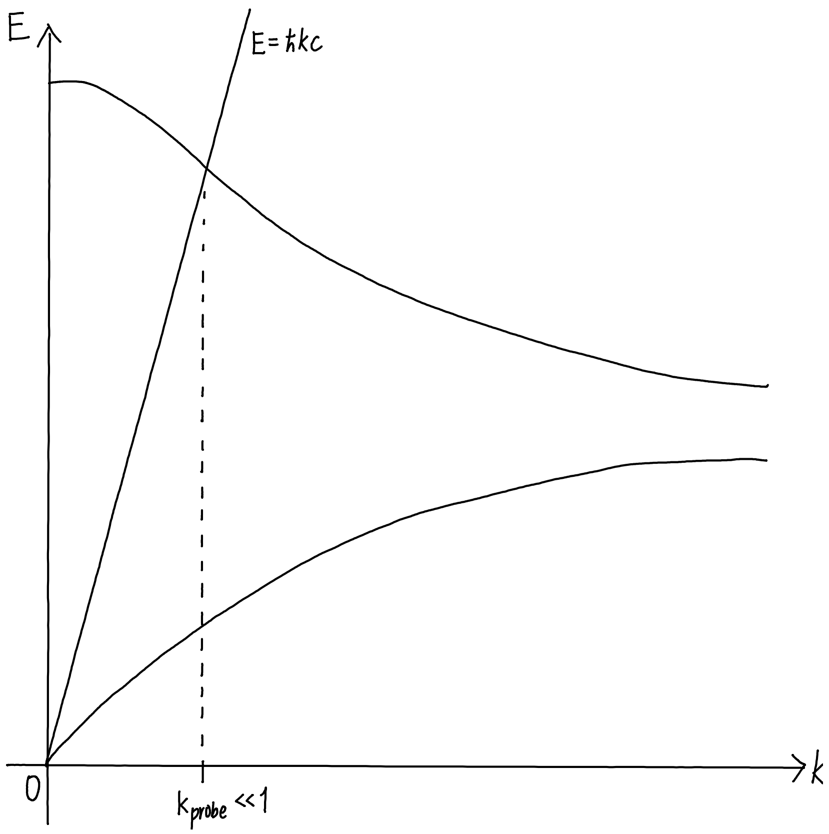
iii. **(TO EXPAND)** $\alpha = \beta = \frac{1}{2}???$

(d) i. From c we have $h_p = (h_r - k_r)/2$ and $k_p = (h_r + k_r)/2$:

$$\begin{aligned}
\Rightarrow P_1 &= \left(\frac{1-0}{2}, \frac{1+0}{2}\right) = \left(\frac{1}{2}, \frac{1}{2}\right) \\
P_2 &= \left(\frac{0-0}{2}, \frac{0+0}{2}\right) = (0, 0)
\end{aligned}$$

in the primitive lattice.

ii. For a phonon to be measurable by IR spectroscopy, it needs to be excited by the IR beam, thus the probable mode must have low momentum (i.e. near BZ boundary) due to the light having large dispersion gradient.



iii. **(TO EXPAND)** P_2 is IR active due to the null wavevector?