Midterm 2011: Solutions

P1

a) The unit cell is a rhombohedral prism with rombus ABCD as one of its bases.
The basis vectors

$$\vec{a}_1 = \frac{a}{2}\left(\sqrt{3}\,\hat{x} + \hat{y}\right)$$

$$\vec{a}_2 = \frac{a}{2}\left(-\sqrt{3}\,\hat{x} + \hat{y}\right)$$

$$\vec{a}_3 = c\,\hat{z}$$

b) The volume of the unit cell:

$$V = \left|(\vec{a}_1 \times \vec{a}_2)\cdot \vec{a}_3\right| = \left(\frac{a}{2}\right)^2 c \left|\left[(\sqrt{3}\,\hat{x}+\hat{y})\times(-\sqrt{3}\,\hat{x}+\hat{y})\right]\cdot\hat{z}\right|$$
$$= \frac{\sqrt{3}}{2}\,a^2 c$$

c) Basis vectors of the reciprocal lattice

$$\vec{b}_1 = \frac{2\pi}{V}(\vec{a}_2\times\vec{a}_3) = \frac{2\pi}{\frac{\sqrt{3}}{2}a^2c}\cdot\frac{a}{2}\cdot c\left(-\sqrt{3}\,\hat{x}+\hat{y}\right)\times\hat{z}$$

$$= \frac{2\pi}{a}\left(\frac{\sqrt{3}}{3}\,\hat{x} + \hat{y}\right)$$

$$\vec{b}_2 = \frac{2\pi}{V}(\vec{a}_3\times\vec{a}_1) = \frac{2\pi}{\frac{\sqrt{3}}{2}a^2c}\cdot\frac{a}{2}\cdot c\,\hat{z}\times\left(\sqrt{3}\,\hat{x}+\hat{y}\right)$$

$$= \frac{2\pi}{a}\left(-\frac{\sqrt{3}}{3}\,\hat{x} + \hat{y}\right)$$

$$\vec{b}_3 = \frac{2\pi}{V}(\vec{a}_1\times\vec{a}_2) = \frac{2\pi}{a^2c\frac{\sqrt{3}}{2}}\left(\frac{a}{2}\right)^2\left(\sqrt{3}\,\hat{x}+\hat{y}\right)\times\left(-\sqrt{3}\,\hat{x}+\hat{y}\right)$$

$$= \frac{2\pi}{c}\,\hat{z},$$ The reciprocal unit cell is a prism with a base built on vectors $\vec{b}_1, \vec{b}_2$.

P2

a) $$E(T) = \int \frac{d^3q}{(2\pi)^3}\, \hbar\omega_q \frac{1}{\left(e^{\frac{\hbar\omega_q}{k_B T}} - 1\right)}$$

$$C(T) = \frac{\partial E}{\partial T} = \frac{1}{k_B T^2} \int \frac{d^3q}{(2\pi)^3} (\hbar\omega_q)^2 \frac{e^{\frac{\hbar\omega_q}{k_B T}}}{\left(e^{\frac{\hbar\omega_q}{k_B T}} - 1\right)^2}$$

For $\omega_q = \omega_0 = \text{const}$

$$C(T) = \frac{1}{k_B T^2} (\hbar\omega_0)^2 \frac{\frac{4\pi}{3} q_D^3}{(2\pi)^3} \frac{e^{\frac{\hbar\omega_0}{k_B T}}}{\left(e^{\frac{\hbar\omega_0}{k_B T}} - 1\right)^2}$$

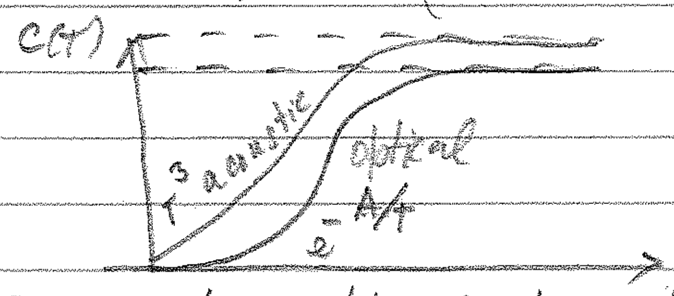
$$= \frac{q_D^3}{6\pi^2} \cdot k_B \left(\frac{\hbar\omega_0}{k_B T}\right)^2 \frac{e^{\frac{\hbar\omega_0}{k_B T}}}{\left(e^{\frac{\hbar\omega_0}{k_B T}} - 1\right)^2}$$

b) For $T \gg \hbar\omega_0/k_B$,

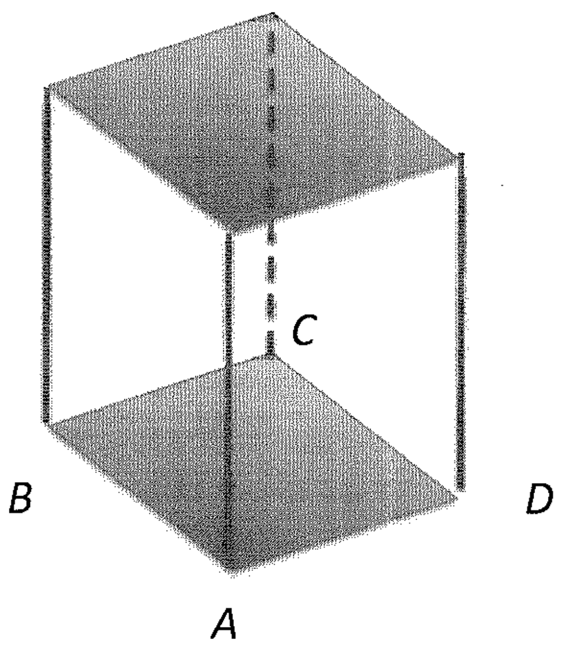
$$C(T) = \frac{q_D^3}{6\pi^2} k_B \left(\frac{\hbar\omega_0}{k_B T}\right)^2 \left(\frac{k_B T}{\hbar\omega_0}\right)^2 = \frac{q_D^3}{6\pi^2} k_B = \text{const}$$

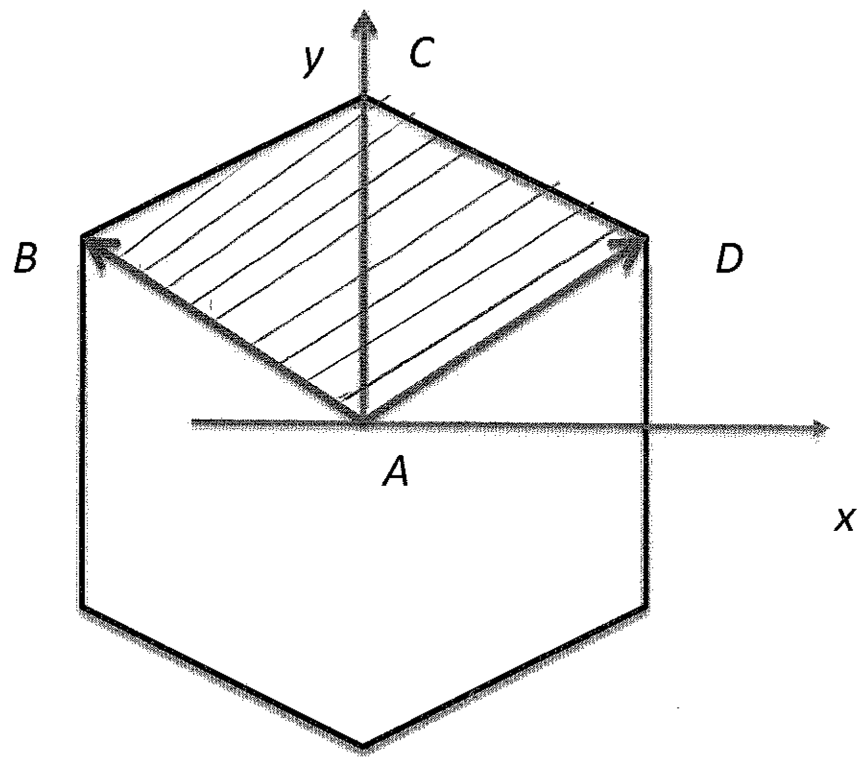
For $T \ll \hbar\omega_0/k_B$

$$C(T) = \frac{q_D^3}{6\pi^2} k_B \left(\frac{\hbar\omega_0}{k_B T}\right)^2 e^{-\frac{\hbar\omega_0}{k_B T}}$$



c) For $T \gg \hbar\omega_0/k_B$, optical phonons' contribution to $C(T)$ is comparable with that of acoustic ones. For $T \ll \hbar\omega_0/k_B$, the optical phonon contr. is exponentially small.


C
B
D
A


y
C
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D
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x