Physics 560A HW 3
Solutions

1) <u>Marder 13.4</u> From lectures 5 + 6, we see that the classical Hamiltonian for phonons in a 3D Bravais lattice can be written

$$H = \sum_{\vec{k},\nu} \left\{ \frac{1}{2m} P^{\dagger}_{\vec{k}\nu} P_{\vec{k}\nu} + \frac{m\omega^2_{\vec{k}\nu}}{2} Q^{\dagger}_{\vec{k}\nu} Q_{\vec{k}\nu} \right\},$$

where $$Q_{\vec{k}\nu} = \frac{\vec{\epsilon}_{\vec{k}\nu}}{\sqrt{N}} \cdot \sum_{l=1}^{N} e^{-i\vec{k}\cdot\vec{R}_l} \vec{X}_l$$

and $$P_{\vec{k}\nu} = \frac{\vec{\epsilon}_{\vec{k}\nu}}{\sqrt{N}} \cdot \sum_{l=1}^{N} e^{i\vec{k}\cdot\vec{R}_l} \vec{P}_l,$$

where $\vec{\epsilon}_{\vec{k}\nu}$ are <u>real eigenvectors</u>

of the 3×3 matrix (2

$$\tilde{C}_{\mu\nu}(\vec{k}) = \sum_{\ell} C_{\mu\nu}(\vec{R}_n - \vec{R}_\ell)\, e^{i\vec{k}\cdot(\vec{R}_n - \vec{R}_\ell)},$$

satisfying $\vec{\epsilon}_{\vec{k}\nu} \cdot \vec{\epsilon}_{\vec{k}\nu'} = \delta_{\nu\nu'}$

and $\sum_{\nu} \vec{\epsilon}_{\vec{k}\nu}\, \vec{\epsilon}_{\vec{k}\nu}^{\,T} = \underline{\mathbb{1}}$.

Creation and annihilation operators are defined in the usual way in terms of the normal coordinates:

$$a_{\vec{k}\nu} = \sqrt{\frac{m\omega_{\vec{k}\nu}}{2\hbar}}\, Q_{\vec{k}\nu} + \frac{i\, P_{-\vec{k}\nu}}{\sqrt{2m\hbar\omega_{\vec{k}\nu}}}$$

$$a^{+}_{\vec{k}\nu} = \sqrt{\frac{m\omega_{\vec{k}\nu}}{2\hbar}}\, Q_{-\vec{k}\nu} - \frac{i\, P_{\vec{k}\nu}}{\sqrt{2m\hbar\omega_{\vec{k}\nu}}}$$

the inverse transformation is

$$Q_{\vec{k}\nu} = \sqrt{\frac{\hbar}{2m\omega_{\vec{k}\nu}}}\left(a_{\vec{k}\nu} + a^{\dagger}_{-\vec{k}\nu}\right)$$

$$P_{\vec{k}\nu} = i\sqrt{\frac{m\hbar\omega_{\vec{k}\nu}}{2}}\left(a^{\dagger}_{\vec{k}\nu} - a_{-\vec{k}\nu}\right)$$

and

$$\vec{x}_{\ell} = \frac{1}{\sqrt{N}}\sum_{\vec{k},\nu} \vec{\epsilon}_{\vec{k}\nu}\, Q_{\vec{k}\nu}\, e^{i\vec{k}\cdot\vec{R}_{\ell}}$$

$$\vec{P}_{\ell} = \frac{1}{\sqrt{N}}\sum_{\vec{k},\nu} \vec{\epsilon}_{\vec{k}\nu}\, P_{\vec{k}\nu}\, e^{-i\vec{k}\cdot\vec{R}_{\ell}}$$

Checking:

$$\vec{x}_{\ell} = \frac{1}{N}\sum_{\vec{k},\nu} \vec{\epsilon}_{\vec{k}\nu}\, e^{i\vec{k}\cdot\vec{R}_{\ell}}\; \vec{\epsilon}_{\vec{k}\nu}\cdot\sum_{\ell'=1}^{N} e^{-i\vec{k}\cdot\vec{R}_{\ell'}}\,\vec{x}_{\ell'}$$

$$\vec{x}_\ell = \sum_{\ell'=1}^{N} \frac{1}{N} \sum_{\vec{k}} e^{i\vec{k}\cdot(\vec{R}_\ell - \vec{R}_{\ell'})} \underbrace{\sum_{\nu} \vec{\epsilon}_{\vec{k}\nu} \vec{\epsilon}_{\vec{k}\nu} \cdot \vec{x}_{\ell'}}_{\vec{x}_{\ell'}}$$

$$\vec{x}_\ell = \sum_{\ell'=1}^{N} \vec{x}_{\ell'} \underbrace{\frac{1}{N} \sum_{\vec{k}} e^{i\vec{k}\cdot(\vec{R}_\ell - \vec{R}_{\ell'})}}_{\delta_{\ell,\ell'}}$$

$$= \vec{x}_\ell \qquad \text{Q.E.D.}$$

similarly for $\vec{P}_\ell$.

[Note: Marder's definitions are almost the same, but I couldn't quite get his to work out.]

b) $\left[a_{\vec{k}\nu}, a^{\dagger}_{\vec{k}'\nu'}\right] = \delta_{\vec{k},\vec{k}'} \delta_{\nu\nu'}$

(to be shown)

$$[a_{\vec{k}\nu}, a^{\dagger}_{\vec{k}'\nu'}] = \frac{-i}{2\hbar}\sqrt{\frac{\omega_{\vec{k}\nu}}{\omega_{\vec{k}'\nu'}}}\,[Q_{\vec{k}\nu}, P_{\vec{k}'\nu'}]$$

$$+ \frac{i}{2\hbar}\sqrt{\frac{\omega_{\vec{k}'\nu'}}{\omega_{\vec{k}\nu}}}\,[P_{-\vec{k}\nu}, Q_{-\vec{k}'\nu'}]$$

Now

$$[Q_{\vec{k}\nu}, P_{\vec{k}'\nu'}] = \frac{1}{N}\sum_{\ell,\ell'} e^{i(\vec{k}'\cdot\vec{R}_{\ell'} - \vec{k}\cdot\vec{R}_\ell)}$$

$$\times\,[\vec{\epsilon}_{\vec{k}\nu}\cdot\vec{x}_\ell,\ \vec{\epsilon}_{\vec{k}'\nu'}\cdot\vec{P}_{\ell'}]$$

$$[\vec{\epsilon}_{\vec{k}\nu}\cdot\vec{x}_\ell,\ \vec{\epsilon}_{\vec{k}'\nu'}\cdot\vec{P}_{\ell'}] =$$

cartesian components

$$\sum_{\alpha=1}^{3}\sum_{\beta=1}^{3} \epsilon^{(\alpha)}_{\vec{k}\nu}\,\epsilon^{(\beta)}_{\vec{k}'\nu'}\,[x^{(\alpha)}_\ell, P^{(\beta)}_{\ell'}]$$

$$= \delta_{\ell\ell'}\,\vec{\epsilon}_{\vec{k}\nu}\cdot\vec{\epsilon}_{\vec{k}'\nu'}\,i\hbar$$

$$[Q_{\vec{k}\nu}, P_{\vec{k}'\nu'}] = i\hbar\,\vec{\epsilon}_{\vec{k}\nu}\cdot\vec{\epsilon}_{\vec{k}'\nu'}\sum_{\ell}\frac{e^{-i(\vec{k}-\vec{k}')\cdot\vec{R}_\ell}}{N}$$

$$= i\hbar\,\delta_{\vec{k}\vec{k}'}\,\vec{\epsilon}_{\vec{k}\nu}\cdot\vec{\epsilon}_{\vec{k}\nu'} = i\hbar\,\delta_{\vec{k}\vec{k}'}\,\delta_{\nu\nu'}$$

$$\Rightarrow \left[a_{\vec{k}\nu}, a^{\dagger}_{\vec{k}'\nu'}\right] = \delta_{\vec{k}\vec{k}'}\,\delta_{\nu\nu'}$$

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2) a) $$N(\omega) = 2\left(\frac{L}{2\pi}\right)^2 \int d^2k\,\theta(\omega-\omega(\vec{k}))$$

$$= \frac{A}{2\pi^2}\,\pi k_{max}^2\,, \quad \omega = v k_{max}$$

$$\Rightarrow N(\omega) = \frac{A}{2\pi}\frac{\omega^2}{v^2}$$

$$\boxed{D(\omega) = \frac{dN}{d\omega} = \frac{A\omega}{\pi v^2}}$$

$$2N = \int_0^{\omega_D} D(\omega)\,d\omega\,,$$ where $N = \#$ of atoms

$$2N = \frac{A}{\pi v^2}\int_0^{\omega_D}\omega\,d\omega = \frac{A\,\omega_D^2}{2\pi v^2}$$

$$\Rightarrow \boxed{\omega_D = v\left(\frac{4\pi N}{A}\right)^{1/2}}$$

b) $$E = \sum_{\vec{k},s} \hbar\omega_s(\vec{k})\left(\langle n_{\vec{k}s}\rangle + \frac{1}{2}\right)$$

$$\boxed{E = \int_0^{\omega_D} d\omega\, D(\omega)\, \hbar\omega \left(\frac{1}{e^{\beta\hbar\omega} - 1} + \frac{1}{2}\right)}$$

c) $$\frac{\partial\langle n\rangle}{\partial T} = \frac{\partial\langle n\rangle}{\partial\beta}\frac{\partial\beta}{\partial T} = -\frac{1}{k_B T^2}\frac{\partial\langle n\rangle}{\partial\beta}$$

$$\frac{\partial\langle n\rangle}{\partial\beta} = -\frac{\hbar\omega\, e^{\beta\hbar\omega}}{\left(e^{\beta\hbar\omega} - 1\right)^2}$$

$$\left.\frac{\partial\langle n\rangle}{\partial T}\right|_V = \frac{\hbar\omega}{k_B T^2}\frac{e^{\beta\hbar\omega}}{\left(e^{\beta\hbar\omega} - 1\right)^2}$$

$$C_V = \int_0^{\omega_D} d\omega\, D(\omega)\, \hbar\omega \left.\frac{\partial\langle n\rangle}{\partial T}\right|_V$$

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$$C_V = \frac{A\hbar^2}{\pi v^2 k_B T^2} \int_0^{\omega_D} d\omega \frac{\omega^3 e^{\beta\hbar\omega}}{(e^{\beta\hbar\omega} - 1)^2}$$

let $x = \beta\hbar\omega$ $\qquad \omega = \frac{k_B T}{\hbar} x$

$$C_V = \frac{A k_B^3 T^2}{\pi \hbar^2 v^2} \int_0^{\beta\hbar\omega_D} dx \frac{x^3 e^x}{(e^x - 1)^2}$$

$$C_V = 4N k_B \left(\frac{T}{\theta}\right)^2 \int_0^{\theta/T} dx \frac{x^3 e^x}{(e^x - 1)^2}$$

where $\theta = \frac{\hbar\omega_D}{k_B}$ = Debye temperature

At low temperatures $(T \ll \theta)$,

$$C_V \simeq 4N k_B \left(\frac{T}{\theta}\right)^2 \underbrace{\int_0^{\infty} dx \frac{x^3 e^x}{(e^x - 1)^2}}_{7.21234}$$

$$\boxed{C_V \simeq 28.849 \times N k_B (T/\theta)^2}$$

3) From problem 1,

$$\vec{X}_\ell = \frac{1}{\sqrt{N}} \sum_{\vec{k},\nu} \vec{E}_{\vec{k}\nu} Q_{\vec{k}\nu} e^{i\vec{k}\cdot\vec{R}_\ell}$$

$$= \frac{1}{\sqrt{N}} \sum_{\vec{k}\nu} \vec{E}_{\vec{k}\nu} \sqrt{\frac{\hbar}{2m\omega_{\vec{k}\nu}}} e^{i\vec{k}\cdot\vec{R}_\ell} \left(a_{\vec{k}\nu} + a^{+}_{-\vec{k}\nu}\right)$$

$$\langle \vec{X}_\ell^{\,2} \rangle = \frac{1}{N} \sum_{\vec{k}\nu} \sum_{\vec{k}'\nu'} \frac{\hbar\, \vec{E}_{\vec{k}\nu}\cdot\vec{E}_{\vec{k}'\nu'}}{\sqrt{4m^2\omega_{\vec{k}\nu}\omega_{\vec{k}'\nu'}}} e^{i(\vec{k}+\vec{k}')\cdot\vec{R}_\ell}$$

$$\times \left\langle \left(a_{\vec{k}\nu} + a^{+}_{-\vec{k}\nu}\right)\left(a_{\vec{k}'\nu'} + a^{+}_{-\vec{k}'\nu'}\right)\right\rangle$$

$$= \left\langle a_{\vec{k}\nu} a^{+}_{-\vec{k}'\nu'} + a^{+}_{-\vec{k}\nu} a_{\vec{k}'\nu'} \right\rangle$$

$$= \delta_{\vec{k},-\vec{k}'}\delta_{\nu\nu'} + \left\langle a^{+}_{-\vec{k}'\nu'} a_{\vec{k}\nu} + a^{+}_{-\vec{k}\nu} a_{\vec{k}'\nu'} \right\rangle$$

$$= \delta_{\vec{k},-\vec{k}'}\delta_{\nu\nu'} \left(1 + \frac{2}{e^{\beta\hbar\omega(\vec{k})} - 1}\right)$$

$$\langle \vec{x}_\ell^{\,2} \rangle = \frac{1}{N} \sum_{\vec{k}\nu} \frac{\hbar\, \vec{\epsilon}_{\vec{k}\nu}\cdot\vec{\epsilon}_{-\vec{k}\nu}}{m\,\omega_{\vec{k}\nu}} \left(\langle n_{\vec{k}\nu} \rangle + \frac{1}{2} \right)$$

$\vec{\epsilon}_{\vec{k}\nu}$ are eigenvectors of $\tilde{C}(\vec{k}) = \tilde{C}(-\vec{k})$

so $\vec{\epsilon}_{\vec{k}\nu} = \vec{\epsilon}_{-\vec{k}\nu}$ and $\vec{\epsilon}_{\vec{k}\nu}\cdot\vec{\epsilon}_{-\vec{k}\nu} = 1$

$$\langle \vec{x}_\ell^{\,2} \rangle = \frac{1}{N} \sum_{\vec{k}\nu} \frac{\hbar}{m\,\omega_{\vec{k}\nu}} \left(\langle n_{\vec{k}\nu} \rangle + \frac{1}{2} \right)$$

$$= \frac{1}{N} \int_0^{\omega_D} d\omega\, \frac{D(\omega)\,\hbar}{m\,\omega} \left(\frac{1}{e^{\beta\hbar\omega} - 1} + \frac{1}{2} \right)$$

$$\langle \vec{x}_\ell^{\,2} \rangle = \frac{A\hbar}{\pi N v^2 m} \int_0^{\omega_D} d\omega \left(\frac{1}{e^{\beta\hbar\omega} - 1} + \frac{1}{2} \right)$$

$$= \underbrace{\frac{A\hbar}{\pi v^2 m}}_{\text{from zero-pt. motion}} + \underbrace{\frac{A\hbar}{\pi N v^2 m} \int_0^{\omega_D} d\omega\, \frac{1}{e^{\beta\hbar\omega} - 1}}_{\text{from thermal excitations}}$$

Expanding the denominator for small frequencies $\frac{\hbar\omega}{k_B T} \ll 1$,

we see that there is a logarithmic divergence at the lower limit of integration

$$\int_0 \frac{d\omega}{\beta\hbar\omega} \to \infty .$$

Thus $\langle \vec{x}_\ell^{\,2} \rangle \to \infty$ for $T > 0$.

(For $T = 0$, there is no frequency such that $\frac{\hbar\omega}{k_B T} \ll 1$, so the issue does not arise, and

$$\langle \vec{x}_\ell^{\,2} \rangle \Big|_{T=0} = \frac{A\hbar}{\pi v^2 m} .)$$