Notes:

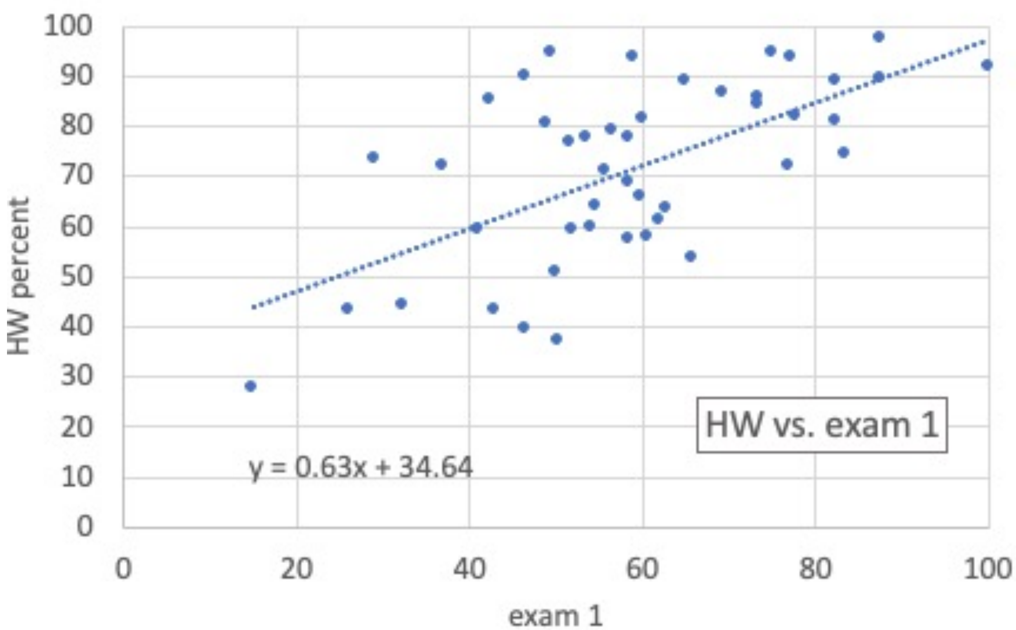
Homework : Set #9 due Thursday not Wednesday. Also note, more on the density of states is included in today's lecture.

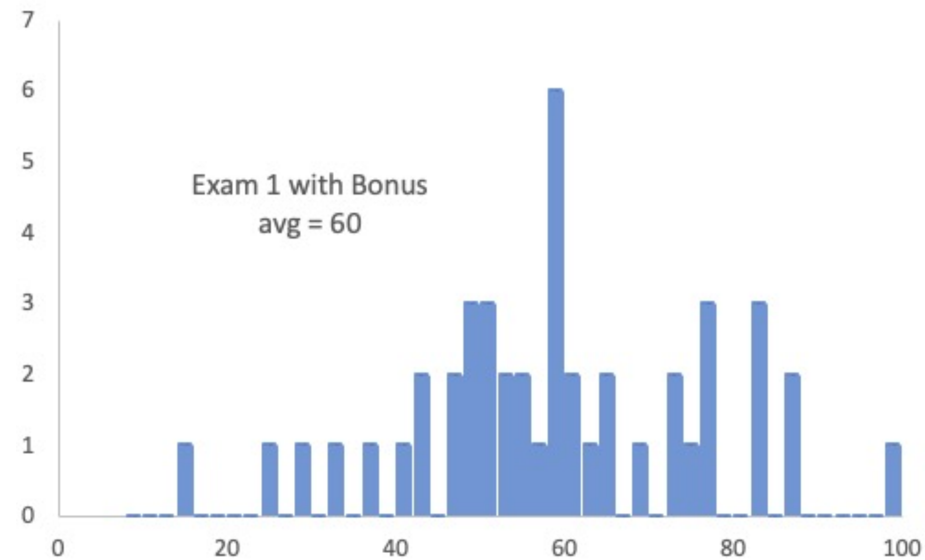
Exam: Results with bonus points, new average = 60.

- I will post solutions later today
- Also I will post adjusted grades on Canvas. (Updated problems are stapled in your exam but I didn't write the adjusted score there, I have the results in a spreadsheet with my bonus algorithm.)
- I had points reversed, sorry, the point totals were 5, 21, 24, 26, 24. I also gave a few more bonus points: 67% of the extra points not 60%).

Notes:

Exam: Results with bonus points, new average = 60.





Homework: Current average is 72. You can also help your cause by volunteering to present one of the HW problems.

Density of states: for summations involving only ω (or E).

phonons

$$U = \sum_{all\ modes} \frac{\hbar\omega_i}{(e^{\beta\hbar\omega_i} - 1)} \Rightarrow 3\int_0^\infty \left(\begin{matrix} \#k\ states \\ in\ (\omega, \omega + d\omega) \end{matrix} \right) \times \frac{\hbar\omega}{(e^{\beta\hbar\omega} - 1)}$$

$$\equiv \int_0^\infty \frac{\hbar\omega D(\omega) d\omega}{(e^{\beta\hbar\omega} - 1)}$$

1) Find # states inside a sphere (octant) in k space: $N(k)$.
   - This includes polarizations.
   - Anisotropic situations: replace sphere by constant-ω surface
2) Convert to ω units: $N(\omega)$.
3) $D(\omega)$ is the derivative, $D(\omega)d\omega = \frac{dN(\omega)}{\mathrm{d}\omega} d\omega$, equal to total # modes in $(\omega, \omega + d\omega)$.

This defines density of states (similar procedure for $D(E)$).

$\Delta k = \frac{\pi}{L}$ -> $V_k = \left(\frac{\pi}{L}\right)^3$ for octant;

$= \left(\frac{2\pi}{L}\right)^3$ for complete sphere

traveling-waves

Result for phonons: $D(\omega) = \frac{3\omega^2 V}{2\pi^2 c^3}$

Phonons:

$$Z = \prod_{all\ modes} Z_i = \prod_{all\ modes} \sum_{n=0}^{\infty} e^{-\beta n \hbar \omega_i} = \prod_{all\ modes} \frac{1}{1 - e^{-\beta \hbar \omega_i}}$$

(not same as all atoms; factor of 3 here)

(Z_i we saw last time)

$$\langle U \rangle = \frac{\partial}{\partial \beta} \ln(Z) = \sum_{all\ modes} \frac{\hbar \omega_i}{(e^{\beta \hbar \omega_i} - 1)}$$

$D(\omega) = \frac{3\omega^2 V}{2\pi^2 c^3}$ use here for sum over ω.

Phonons:

continuum limit

$$\langle U \rangle = \sum_{all\ modes} \frac{\hbar\omega_i}{(e^{\beta\hbar\omega_i}-1)} \Longrightarrow \int_0^{\omega_{max}} \frac{\hbar\omega D(\omega) d\omega}{(e^{\beta\hbar\omega}-1)} = \int_0^{\omega_D} \frac{3V\hbar\omega^3 d\omega}{2\pi^2 c^3 (e^{\beta\hbar\omega}-1)}$$

Phonons:

$$D(\omega) = \frac{3\omega^2 V}{2\pi^2 c^3}$$

continuum limit

$$\langle U \rangle = \sum_{all\ modes} \frac{\hbar\omega_i}{(e^{\beta\hbar\omega_i} - 1)} \Longrightarrow \int_0^{\omega_{max}} \frac{\hbar\omega D(\omega) d\omega}{(e^{\beta\hbar\omega} - 1)} = \int_0^{\omega_D} \frac{3V\hbar\omega^3 d\omega}{2\pi^2 c^3 (e^{\beta\hbar\omega} - 1)}$$

$$\langle U \rangle = \frac{V\pi^2 (kT)^4}{10(\hbar c)^3}$$

low T only
and note, c = speed of sound (not light)

Debye Theory:

- Modes cut off uniformly in all directions: maximum $k = k_D$ on sphere.
- Assume uniform speed of sound, doesn't change at high frequencies.
- Disregard anisotropy, e.g. for layered crystals, etc.

Phonons:

continuum limit

$$\langle U \rangle = \sum_{all\ modes} \frac{\hbar\omega_i}{(e^{\beta\hbar\omega_i} - 1)} \Longrightarrow \int_0^{\omega_{max}} \frac{\hbar\omega D(\omega) d\omega}{(e^{\beta\hbar\omega} - 1)} = \int_0^{\omega_D} \frac{3V\hbar\omega^3 d\omega}{2\pi^2 c^3 (e^{\beta\hbar\omega} - 1)}$$

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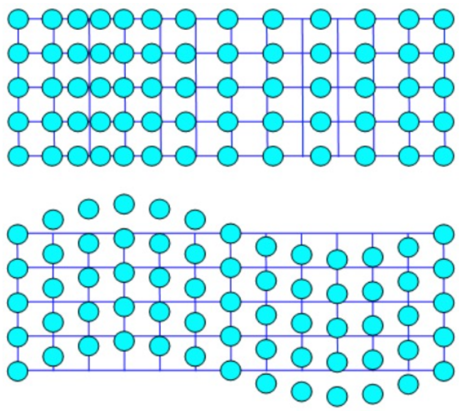
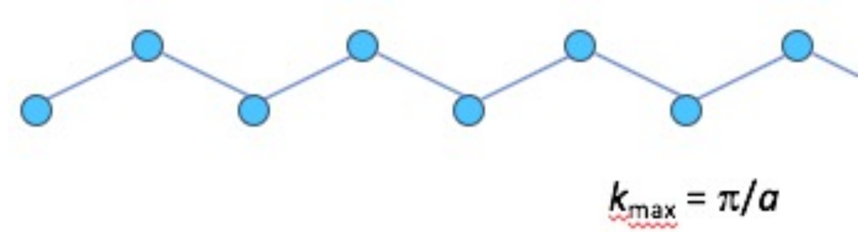
Result: $\omega_D = c\left(6\pi^2 \frac{N}{V}\right)^{1/3}$ need this for solutions at general T

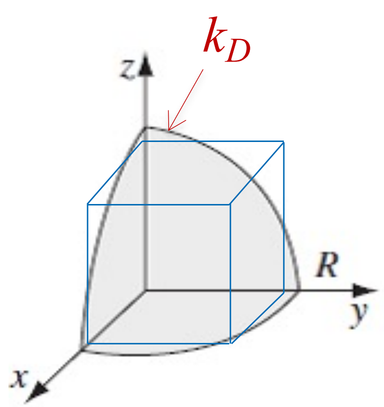
Phonons mode counting:





Debye Theory ("Debye approximation"):

- Modes cut off uniformly in all directions: maximum $k = k_D$ on sphere.
- Assume constant speed of sound, doesn't change at high frequencies.
- Disregard anisotropy, e.g. for layered crystals, etc.
- Even in simple crystal geometries (cubic), cutoff is really a polyhedron in k space (this is the "Brillouin zone"; Debye approximation neglects this.



Polyhedron with 3N modes;
Sphere same volume, also 3N modes.

$\omega_D \equiv k_D c$ Debye frequency

$\Theta_D \equiv \hbar\omega_D / k_B$ Debye temperature

Result:

$$\omega_D = c\left(6\pi^2 \frac{N}{V}\right)^{1/3}$$

Phonons: combining,

continuum limit

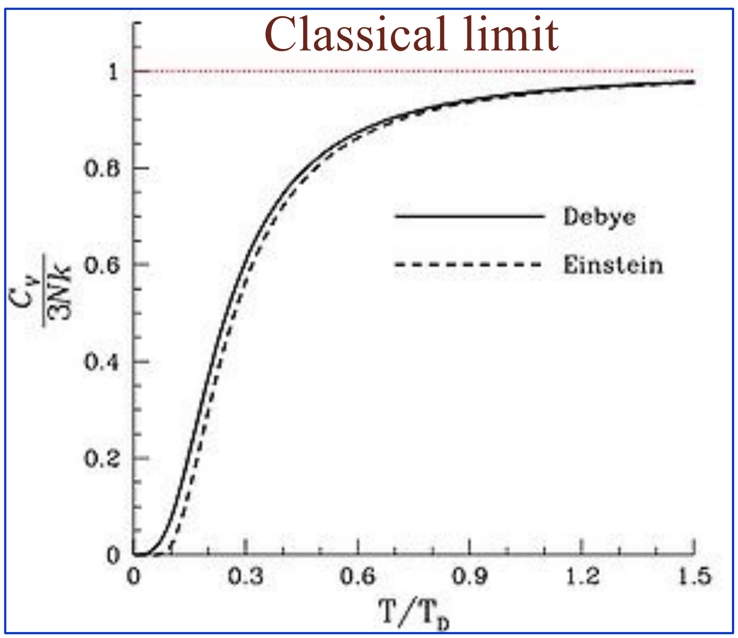
$$\langle E \rangle = \sum_{all\ modes} \frac{\hbar\omega_i}{(e^{\beta\hbar\omega_i} - 1)} \Rightarrow \int_0^{\omega_D} \frac{3V\hbar\omega^3 d\omega}{2\pi^2 c^3 (e^{\beta\hbar\omega} - 1)}$$

$$\langle E \rangle = \frac{V\pi^2 (kT)^4}{10(\hbar c)^3}$$

low T limit (*exact result*)
c = speed of sound (or *directional average*)

$$\text{Low-}T\ C_V = \frac{12}{5} N\pi^4 k_B \left(\frac{T}{\Theta_D}\right)^3 \qquad \Theta_D = \frac{\hbar\omega_D}{k_B} = \frac{\hbar c}{k_B}\left(\frac{6\pi^2 N}{V}\right)^{1/3}$$

Debye Temperature



higher T : can solve integral numerically. Generally good agreement, Debye theory commonly used to model thermal behavior of solids.

Copper Θ_D = 315 K
Lead Θ_D = 88 K
Diamond Θ_D = 1860 K

Debye approximation: Commonly used as measure of phonon behavior (even when "real" behavior can be obtained)

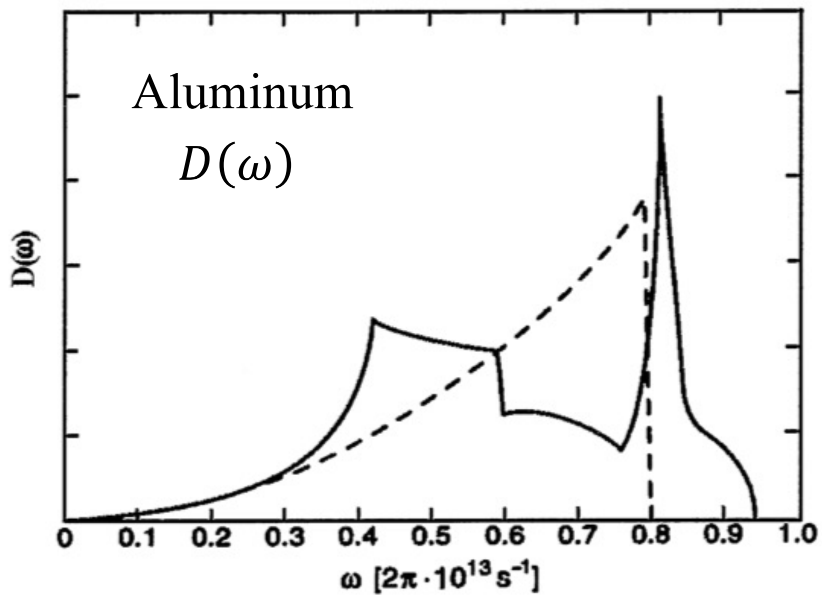
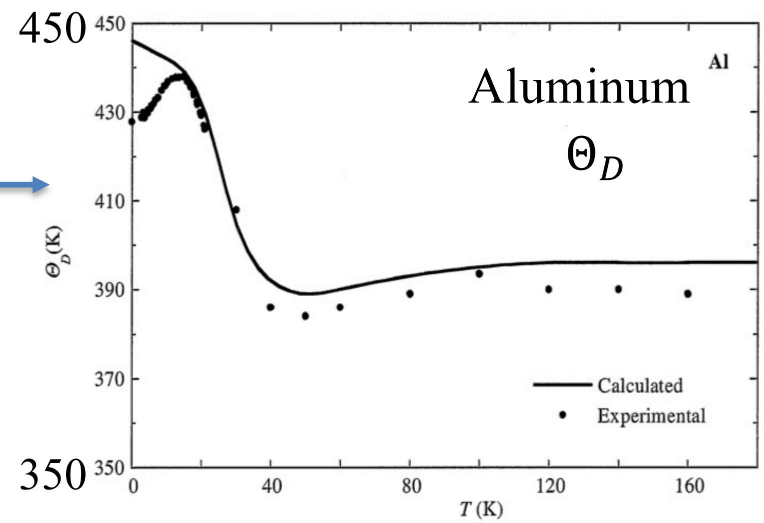
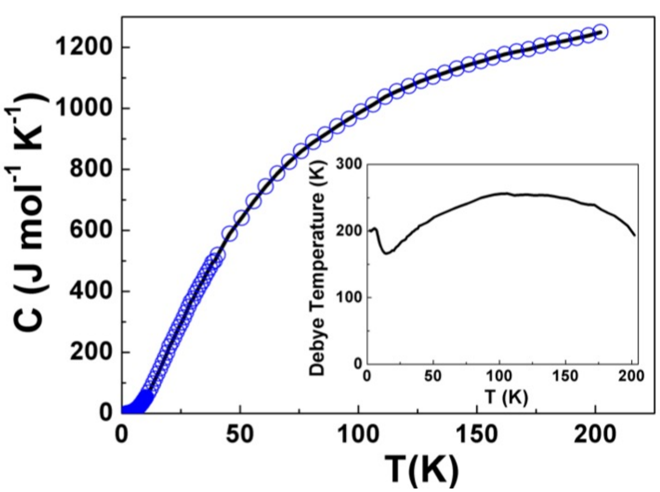
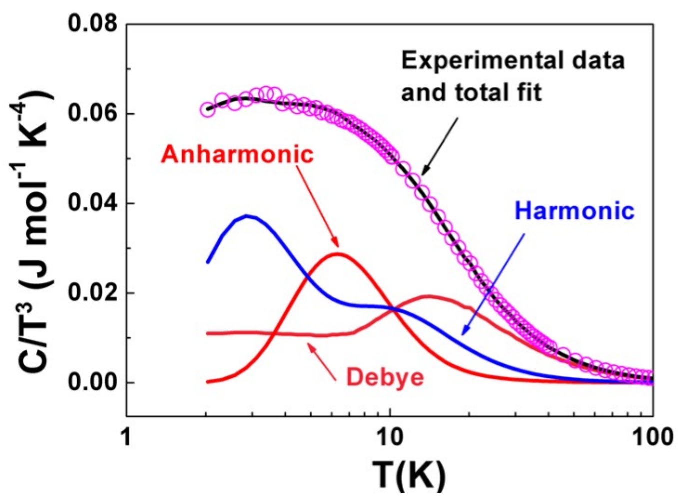


Figure 2.9. The density of frequency modes for Al at 300K (solid line) obtained by Walker [**30**] and that for the Debye model (dashed lines)



from "The Specific Heat of Matter at Low Temperatures" [Tari, 2003].





X Zheng et al. Phys. Rev. B 85, 214304 (2012) [my lab]:

<u>Specific heat</u> of thermoelectric crystal.

Density of states:

$$3\times\begin{pmatrix} \#k\ states \\ in\ (\omega, \omega + d\omega) \end{pmatrix} \equiv D(\omega)$$ *recall for phonons*:

1) Find # states inside a sphere (octant) in k space: $N(k)$.
   • include 3 polarizations.
2) Convert to ω units: $N(\omega)$.
3) $D(\omega)$ is the derivative, $D(\omega)d\omega = \frac{dN(\omega)}{\mathrm{d}\omega}d\omega$, equal to total # modes in $(\omega, \omega + d\omega)$.

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other systems: **Ideal gas of electrons**

1) Find # states inside a sphere (octant) in k space: $N(k)$. (same)
   • include 2 spins.
2) Convert to ε units: $N(\varepsilon)$. ← $(\varepsilon = \frac{\hbar^2 k^2}{2m})$
3) $D(\varepsilon)$ is the derivative, $D(\varepsilon)d\varepsilon = \frac{dN(\varepsilon)}{\mathrm{d}\varepsilon}d\varepsilon$, equal to total # modes in $(\varepsilon, \varepsilon + d\varepsilon)$.

$\Delta k = \frac{\pi}{L}$ -> $V_k = \left(\frac{\pi}{L}\right)^3$ for octant;

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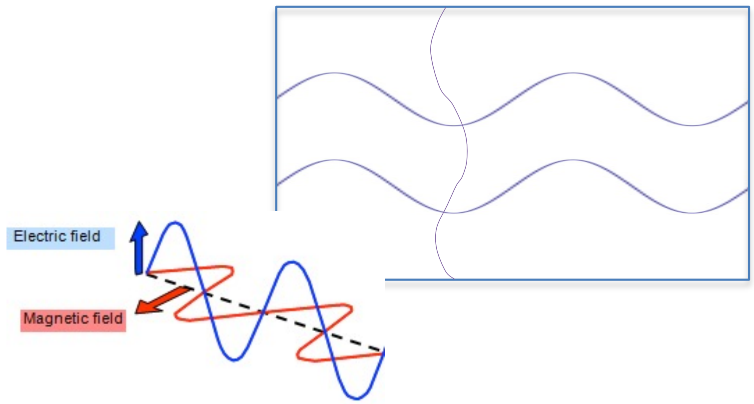
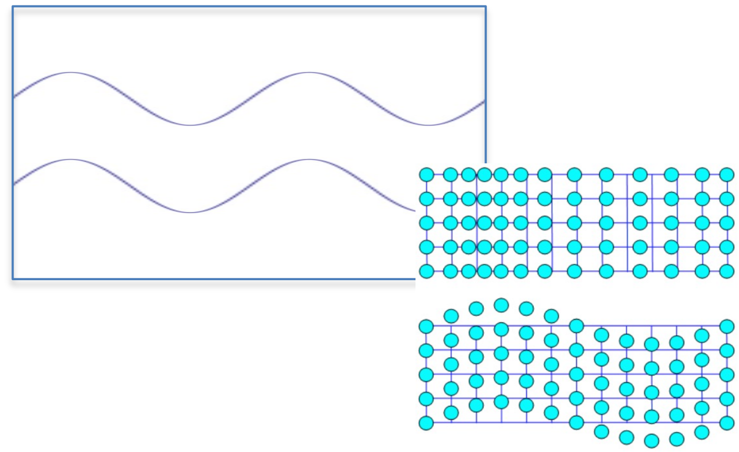
3) $D(\varepsilon)$ is the derivative, $D(\varepsilon)d\varepsilon = \frac{dN(\varepsilon)}{d\varepsilon}d\varepsilon$, equal to total # modes in $(\varepsilon, \varepsilon + d\varepsilon)$.

Result: $D(\varepsilon) = \frac{2V}{(4\pi^2)}\left(\frac{2m}{\hbar^2}\right)^{3/2}\sqrt{\varepsilon}$

- Similar procedure for relativistic gas (HW)
- For the ionization HW problem 6, previously I didn't include *spin* in the multiplicity of states. Using the result above you should arrive within a *factor of 2* vs. the prior result.
- Classical partition function can be calculated this way. Last week we did so with momentum integration, this is easier.
- Ch. does not give $D(\varepsilon)$ with energy units, this appears later chapter 18.

Photons vs. Phonons recall:





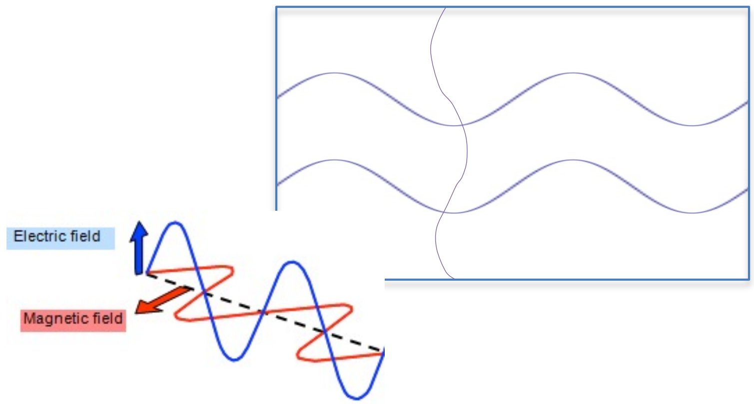
Photons:

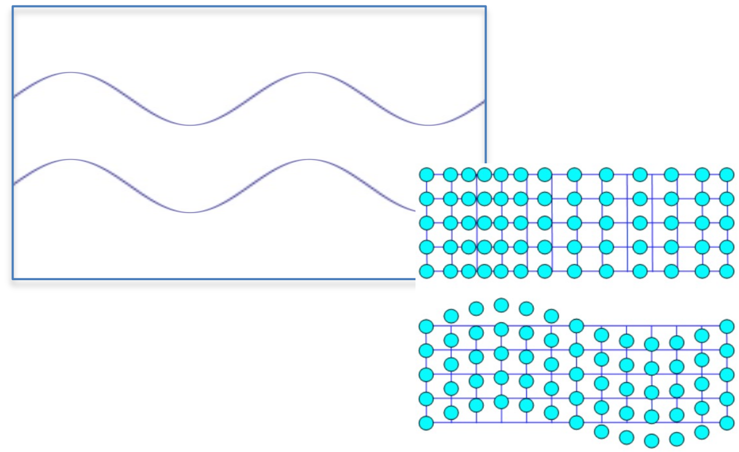
- Cavity modes
- 2 polarizations
- $\omega = kc$.
- Extend to $\omega \to \infty$.
- $e^{-i\vec{k}\cdot\vec{r}-\omega t}$ free space solution
- Bose statistics ($\mu = 0$).
- Energies quantized, $\hbar\omega(n + \frac{1}{2})$.
- Speed of light: c.

Phonons:

- elastic (standing) waves
- **3 polarizations**
- $\boldsymbol{\omega \cong kc}$**, exact for low** $\boldsymbol{k}$
- **Bounded: N values of k.**
- $e^{-i\vec{k}\cdot\vec{r}-\omega t}$ [or $\sin(\vec{k}\cdot\vec{r})\sin(\omega t)$]
- Bose statistics ($\mu = 0$).
- Energies quantized, $\hbar\omega(n + \frac{1}{2})$.
- Speed of sound: c

Photons vs. Phonons recall:





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- Speed of light: c.

$$D(\omega) = \frac{2}{3}\times\frac{3\omega^2 V}{2\pi^2 c^3} = \frac{\omega^2 V}{\pi^2 c^3}$$

Phonons:

- elastic (standing) waves
- **3 polarizations**
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- Energies quantized, $\hbar\omega(n+\frac{1}{2})$.
- Speed of sound: c

$$D(\omega) = \frac{3\omega^2 V}{2\pi^2 c^3}$$

Phonons vs Photons we also saw before:

- Liquids and non-crystal solids: have similar modes.
- **Einstein**: independent 3D oscillators, same ω_o.
- **Debye**: Phonons are normal modes in a *connected* harmonic lattice.
- Debye-theory solutions identical to sound waves , $\omega = kc$ (exact in low-frequency limit); also map onto blackbody-radiation photons.
- Except: mode counting requires finite number of phonon modes, and 3 polarizations, not 2.