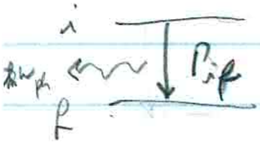
Lecture #18: Equilibrium distribution of Fermions and Bosons, density of states.

Fermi's golden rule, from time-dependent perturbation theory.

Due to perturbation V_{int} (e.g. electron-phonon or electron-photon interaction)
(See $\langle + \rangle$ for a derivation):



$$\Gamma_{if} = \frac{2\pi}{\hbar}\left|\langle f | V_{int} | i\rangle\right|^2 D(E_f)$$

or

$E_i = E_f + \hbar\omega_{ph}$

$$\Gamma_{if} = \frac{2\pi}{\hbar}\left|\langle f | V_{int} | i\rangle\right|^2 \underbrace{\delta(E_f - E_i)}_{\text{Conservation of energy.}}$$

(assuming that the actual rate will be an integration over this).

For example,

$V_{int} = \sum_{k,k'} A_{kk'} a^{\dagger}_{k'} a_k$. Suppose the system is at $|i\rangle = |N_k = N_i\rangle$, a Fock state.
The transition rate into another Fock state $|f\rangle = |N_{k'} = N_f\rangle$ is given by:

$$\Gamma_{i\to f} = \frac{2\pi}{\hbar}\left|\underbrace{\langle f | \sum_{k,k'} A_{kk'} a^{\dagger}_{k'} a_k | i\rangle}\right|^2 \delta(E_f - E_i)$$

$= \sqrt{N_i}\sqrt{N_f + 1}\, A_{if}$ for Bosons
$= \sqrt{N_i}\sqrt{1 - N_f}\, A_{if}$ for Fermions

$$\Gamma_{i\to f} = \frac{2\pi}{\hbar}|A_{if}|^2 N_i \begin{cases} (1 + N_f) & \text{for Bosons} \\ (1 - N_f) & \text{for Fermions} \end{cases}$$

"stimulated emission" of Bosons: The more photons there are in the final state, the faster is the transition into it.

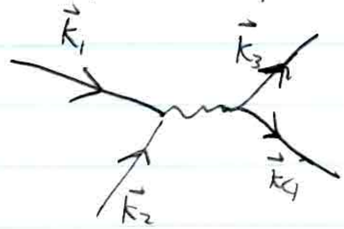
(Opposite for Fermions)

What is the equilibrium occupation $f(\epsilon_k) = \langle \hat{N}_k \rangle$ for Bosons and Fermions?

Systems equilibrate because of interparticle interactions,

$$V_{int} = \frac{1}{2} \sum_{k_1, k_2, k_3} U_{k_1, k_2, k_3, k_4} \, a^\dagger_{k_4} a^\dagger_{k_3} a_{k_2} a_{k_1}$$

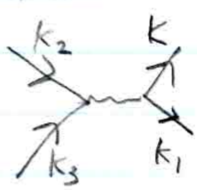
Need only to sum over k_1, k_2, k_3 because of Conservation of mom.: $\vec{k}_1 + \vec{k}_2 = \vec{k}_3 + \vec{k}_4$

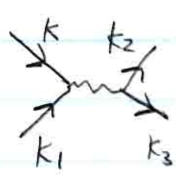


Feynman diagram for the interaction

Focus on a particular state, say k.

$$\frac{dN_k}{dt} = \left[+ \sum_{k_2, k_3, k_1} N_{k_2} N_{k_3} (1 \pm N_{k_1})(1 \pm N_k) - \sum N_k N_{k_1} (1 \pm N_{k_2})(1 \pm N_{k_3}) \right] \times \text{Const}$$





$$\frac{dN_k}{dt} = 0 \Rightarrow^{(*)} f(\epsilon_{k_2}) f(\epsilon_{k_3}) \left[1 \pm f(\epsilon_{k_1})\right]\left[1 \pm f(\epsilon_k)\right] = f(\epsilon_k) f(\epsilon_{k_1}) \left[1 \pm f(\epsilon_{k_2})\right] \times \left[1 \pm f(\epsilon_{k_3})\right]$$

and $\boxed{\epsilon_k + \epsilon_{k_1} = \epsilon_{k_2} + \epsilon_{k_3}}$.

"detailed balance": At equilibrium, amount going out equals amount going in!

Can be proven that

$\Rightarrow$ Only $f(\epsilon) = \dfrac{1}{e^{\alpha + \beta\epsilon} \mp 1}$ satisfies this. $\Longrightarrow$ See bottom of next page

$-$: Bosons, $+$: Fermions

Find α and β from

$$N = \sum_k f(\epsilon_k) = \int f(\epsilon) D(\epsilon) d\epsilon$$

$$U = \sum_k \epsilon_k f(\epsilon_k) = \int \epsilon f(\epsilon) D(\epsilon) d\epsilon$$

or in the limit $\alpha >> 1$: $f(\epsilon) \simeq e^{-(\alpha + \beta\epsilon)}$ $\begin{cases} \alpha = \frac{-\mu}{k_B T} \\ \beta = \frac{1}{k_B T} \end{cases}$

equate to the classical dist:

$f(\epsilon) = e^{-\beta\epsilon} e^{\frac{\mu}{kT}} \Rightarrow$

$$\Rightarrow f(\epsilon) = \frac{1}{e^{\frac{(\epsilon-\mu)}{k_B T}} \mp 1}$$

This derivation gives an explanation of why Bosons have the $-$ and Fermions have the $+$ in the distribution func!

Define $f(\epsilon) = \dfrac{1}{g(\epsilon) \mp 1}$ and plug into $(*)$ to get:

$$\boxed{g(\epsilon_k) g(\epsilon_{k1}) = g(\epsilon_{k2}) g(\epsilon_{k3})} \Rightarrow \ln[g(\epsilon_k)] + \ln[g(\epsilon_{k1})] = \ln[g(\epsilon_{k2})] + \ln[g(\epsilon_{k3})]$$

+ Conservation of energy: $\boxed{\epsilon_k + \epsilon_{k1} = \epsilon_{k2} + \epsilon_{k3}}$

Check that these two equations are satisfied simultaneously only if $\ln[g(\epsilon)] = (\alpha + \beta\epsilon)$ with α and β constants.

$$\Rightarrow g(\epsilon) = e^{\alpha + \beta\epsilon}$$

(4)

Nov 8

Energy density for phonons and photons

$$U = \int_0^\infty dE \cdot E\, f(E)\, D(E) \quad , \qquad f(E) = \frac{1}{e^{\frac{\hbar\omega}{k_BT}} - 1}$$

because $\mu = 0$ (Lagrange multipl for # of particles) and photons and phonons are Bosons!

$$C_V = \left(\frac{\partial U}{\partial T}\right)_V$$

Density of states per mode: $D(E)\,dE = \dfrac{d^3k}{\frac{(2\pi)^3}{V}} = \dfrac{4\pi k^2 dk}{\frac{8\pi^3}{V}}$

$$= \frac{V}{2\pi^2} \frac{k^2}{|\vec{\nabla}_k E|} dE$$

$$\boxed{D(E) = \frac{V}{2\pi^2} \frac{k^2}{\left|\frac{dE}{dk}\right|}}$$

For $E = \hbar\omega = \hbar v |\vec{k}|$:

$$D(E) = \frac{V}{2\pi^2} \frac{E^2}{(\hbar v)^2} \frac{1}{(\hbar v)}$$

For photons, $v = \frac{c}{n}$ and 2 polarizations : $\boxed{D_{\text{photons}}(E) = \dfrac{V n^3}{\pi^2 (\hbar c)^3} E^2}$

For phonons, 3 polarizations : $\boxed{D_{\text{phonons}}(E) = \dfrac{3V}{2\pi^2 (\hbar v)^3} E^2}$

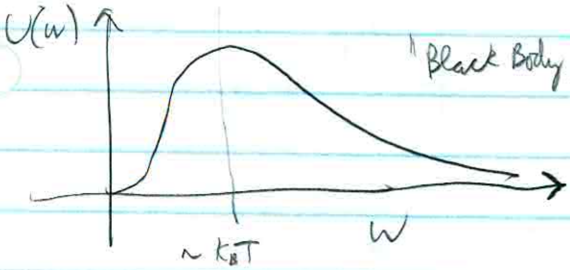
Planck energy density in cavity:

$$U(\omega)\,d\omega = \hbar\omega \frac{1}{e^{\frac{\hbar\omega}{k_BT}}-1}\, D_{photon}(\hbar\omega) = \frac{1}{e^{\frac{\hbar\omega}{kT}}-1}\left(\frac{V n^3}{\pi^2 c^3}\right)\omega^3$$

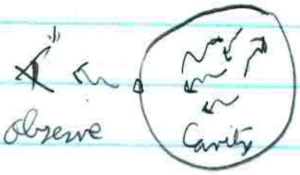
$$U_{TOTAL} = \int_0^\infty U(\omega)\,d\omega = \left(\frac{V n^3}{\pi^2 c^3}\right)\int_0^\infty d\omega \,\frac{\omega^3}{e^{\frac{\hbar\omega}{kT}}-1} = \frac{V n^3}{\pi^2 c^3}\left(\frac{k_BT}{\hbar}\right)^4 \underbrace{\int_0^\infty dx\, \frac{x^3}{e^x-1}}_{=\frac{\pi^4}{15}}$$

$x = \frac{\hbar\omega}{kT}$

$$\boxed{U_{Total} \propto T^4}$$ stefan-Boltzmann law



"Black Body radiation": E.g., fit this to a star to determine the temperature of the star.



Heat capacity for phonons, Debye model

Phonons are different than photons in the sense that they are a discrete lattice of atoms, hence they have a cut off in K: $K_{max} \sim \frac{\pi}{a}$.

Debye model is to assume a sharp cut-off, $K = K_{Debye} \equiv K_D$.

Therefore,
$$D_{phonons}(\epsilon) = \begin{cases} \frac{3V}{2\pi^2(\hbar v)^3} E^2 & \text{if } E < \hbar v K_D \\ 0 & \text{if } E > \hbar v K_D \end{cases}$$

⑥

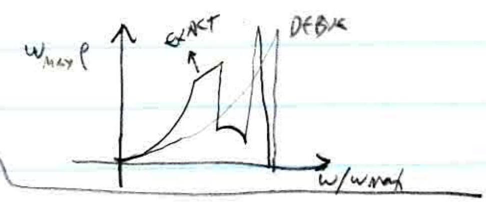
To find k_D, equate $N_{atoms} = \dfrac{\frac{4}{3}\pi k_D^3}{\frac{(2\pi)^3}{V}} = \dfrac{V}{6\pi^2} k_D^3 \Rightarrow \boxed{k_D = 6\pi^2\left(\dfrac{N_{atoms}}{V}\right)}$

$$U_{ph} = 3\int_0^{k_D} \frac{4\pi k^2\, dk}{\frac{(2\pi)^3}{V}} (\hbar v k) \frac{1}{e^{\frac{\hbar v k}{kT}} - 1}$$

At low T, we can extend this integral to ∞ because $\dfrac{\hbar v k_D}{kT} >> 1$:

Peter Young's website

PHONON DENSITY OF STATES FOR MONATOMIC FCC (SPRING MODEL) $\omega_{max} = 2\sqrt{2K/M}$



$$U_{ph} = \int_0^\infty dk \frac{k^3}{e^{\frac{\hbar v k}{kT}} - 1} \left(\frac{12\pi V \hbar v}{8\pi^3}\right)$$

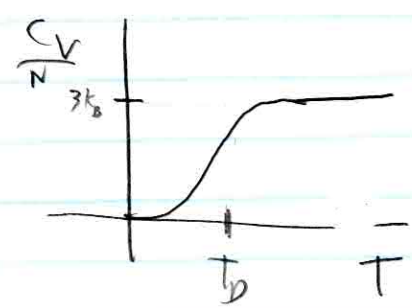
$$= \left(\frac{kT}{\hbar v}\right)^4 \left(\frac{3V\hbar v}{2\pi^2}\right) \frac{\pi^4}{15} \propto T^4$$

$$\Rightarrow C_v = \left(\frac{\partial U}{\partial T}\right)_V \propto T^3 \quad // \quad \left(T << T_{Debye} = \frac{\hbar v k_D}{k_B}\right)$$

At high T, $T >> T_{Debye}$:

$$U_{ph} = 3V \int_0^{k_D} \frac{dk}{\cancel{8\pi^3}\ 2\pi^2} \cancel{4\pi\hbar v} \frac{k^{\cancel{3}\,2}}{\frac{\cancel{\hbar v k}}{k_B T} + O\left(\frac{1}{T}\right)^2} = \frac{3Vk_BT}{2\pi^2}\int_0^{k_D} dk\, k^2$$

$$= \frac{3Vk_BT}{2\pi^2}\frac{k_D^3}{3} = 3k_BT\underbrace{\left(\frac{Vk_D^3}{6\pi^2}\right)}_{N_{atom}}$$



$U_{ph} = 3N_{atom}k_BT$ (6N degrees of freedom, 3N x and 3N p) "Equipartition thm"

$\boxed{\dfrac{C_v}{N} = 3k_B}$ "Dulong-Petit law"

$\Rightarrow$ Show plots of phonon density of states for real materials
prepare slides