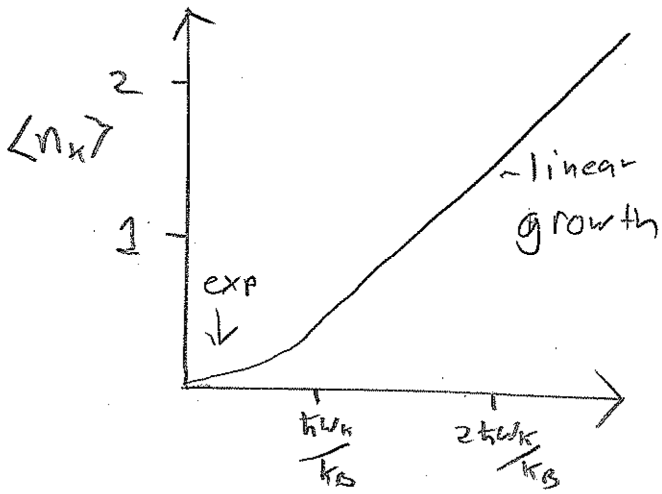
Day 8

Let's define an average occupancy $\langle n_k \rangle$, given by Bose-Einstein statistics:

$$\langle n_k \rangle = \frac{1}{e^{\hbar\omega_k / k_B T} - 1}$$



When $T < \frac{\hbar\omega_k}{k_B}$ phonon population is exponentially suppressed or frozen out.

The total energy in the system is now:

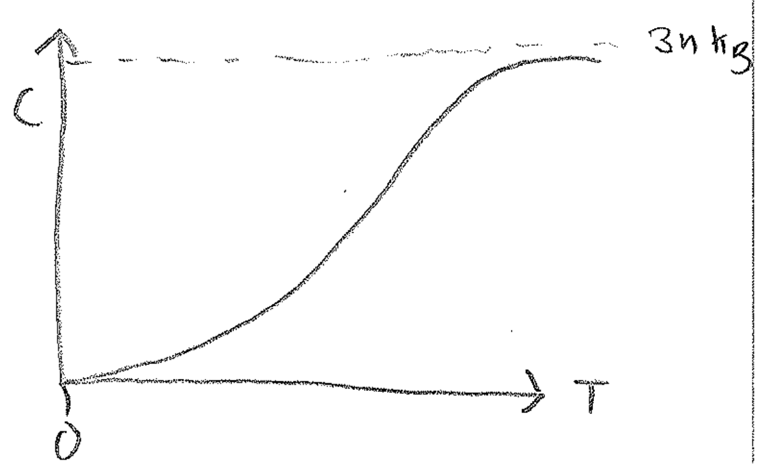
$$U(T) = \sum_{\text{all } k} 3\hbar\omega_k \left(\langle n_k \rangle + \tfrac{1}{2}\right)$$

Compare vs. $U = 3n k_B T$ (Classical mech)

A materials <u>heat capacity</u> is defined as:

$$C \equiv \frac{dU}{dT}$$

$$= \sum_k 3\hbar\omega_k \frac{d\langle n_k \rangle}{dT}$$



Example: Questions on thermal properties

(1) How many phonons populate the highest frequency acoustic mode in diamond?

$$\omega_{max} = \omega_D = 2\sqrt{\alpha/m}\ , \quad T = 300\,K\ , \quad \alpha = 20\ N/m$$

$$m = 12 \cdot 2 \times 10^{-27}\ kg$$

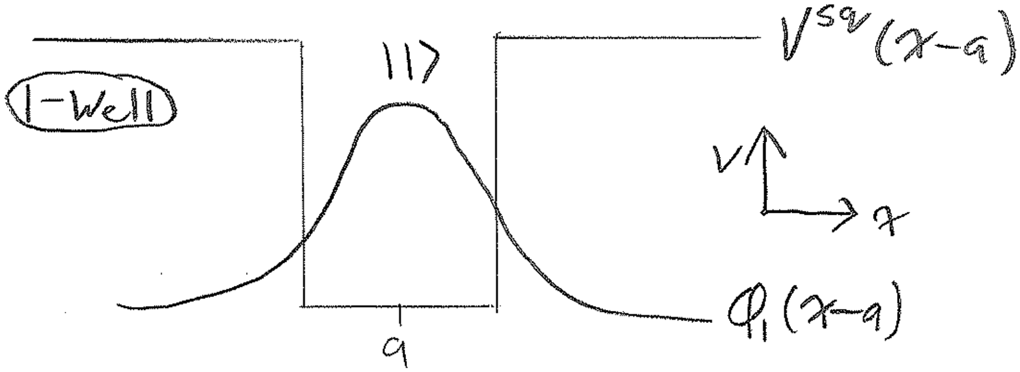
$$\langle n_k \rangle = \frac{1}{\exp(\hbar\omega_D/(k_B 300)) - 1} = ?$$

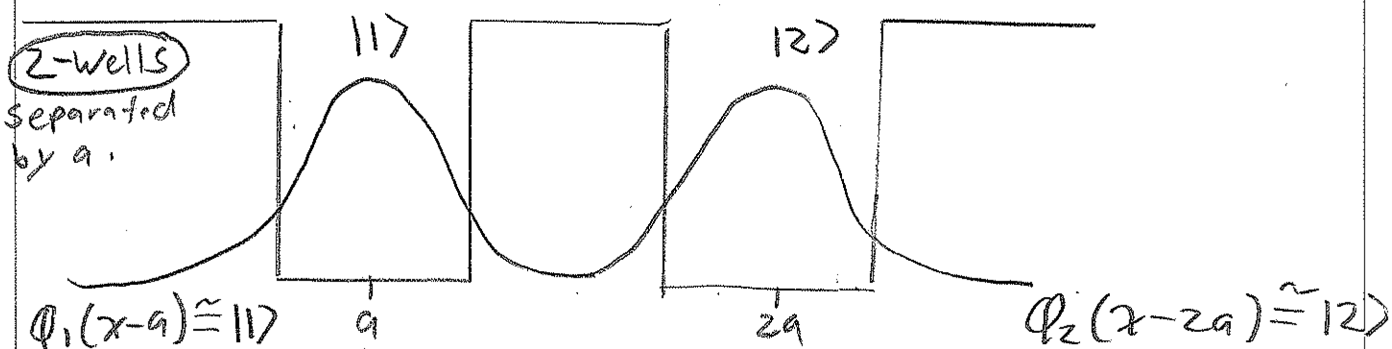
(2) At what temperature does the highest frequency mode have $\langle n_k \rangle = \frac{1}{2}$?

$$\frac{1}{2} = \frac{1}{e^{\hbar\omega_D/k_B T} - 1} = ?\ ,$$ solve for T

Ch. 15.1 Electronics in solids (Mc Intyre)

Let electrons be confined to a periodic finite square well:





Assume $|1\rangle$ and $|2\rangle$ form a nearly orthogonal basis such that:

$$V(x) = V^{sq}(x-a) + V^{sq}(x-2a)$$

What is $|\psi\rangle$? $\Rightarrow$ apply "Linear Combination of Atomic Orbitals" (LCAO) approx that says:

$$|\psi\rangle \cong c_1 \varphi(x-a) + c_2 \varphi(x-2a)$$

$$H|\psi\rangle = E|\psi\rangle \Rightarrow H \begin{bmatrix} c_1 \\ c_2 \end{bmatrix} = E \begin{bmatrix} c_1 \\ c_2 \end{bmatrix}$$

$H_{11} = \langle 1 | \hat{H} | 1 \rangle$, etc.

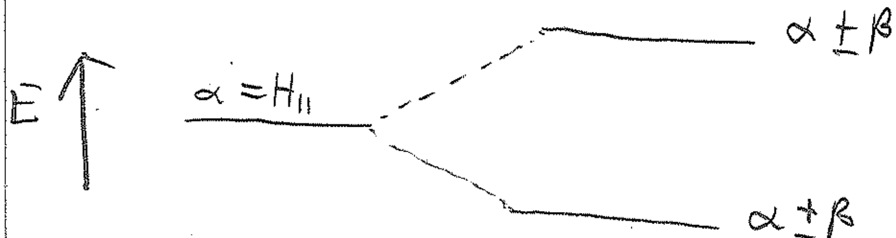
$$H = \begin{bmatrix} \langle 1|\hat{H}|1\rangle & \langle 1|\hat{H}|2\rangle \\ \langle 2|\hat{H}|1\rangle & \langle 2|\hat{H}|2\rangle \end{bmatrix} \equiv \begin{bmatrix} \alpha & \beta \\ \beta & \alpha \end{bmatrix},$$

why does $H_{12} = H_{21}$??

Excercise: solve $H|\Psi\rangle = E|\Psi\rangle$ for $E = \lambda$

$$0 = \det(H - EI)$$
$$= (\alpha - E)^2 - \beta^2$$

$$\therefore \quad E = \alpha \pm \beta$$



is $\beta > 0$ or < 0? we don't know yet!

What about the eigen-states?

orthonormal basis

Case 1: $E = \alpha + \beta \implies \begin{bmatrix} c_1 \\ c_2 \end{bmatrix} = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 1 \end{bmatrix}$

$$(H - E_+ I)\begin{bmatrix} c_1 \\ c_2 \end{bmatrix} = \begin{bmatrix} -\beta & \beta \\ \beta & -\beta \end{bmatrix}\begin{bmatrix} c_1 \\ c_2 \end{bmatrix} = 0 \implies c_1 = c_2$$

OR $|\Psi_+\rangle = \frac{1}{\sqrt{2}}(|1\rangle + |2\rangle)$

Case 2: $E = \alpha - \beta$

$$\begin{bmatrix} \beta & \beta \\ \beta & \beta \end{bmatrix}\begin{bmatrix} c_1 \\ c_2 \end{bmatrix} = 0 \implies c_1 = -c_2$$

or $|\psi_-\rangle = \frac{1}{\sqrt{2}}\left(|1\rangle - |2\rangle\right)$

problem set: do the same thing for a 3×3
matrix of 3 quantum wells.