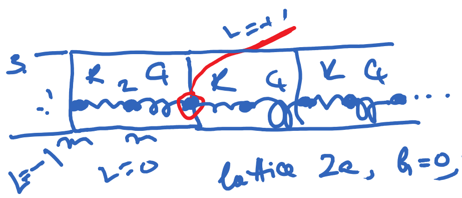
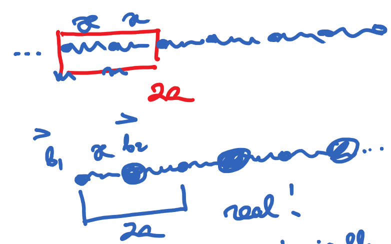
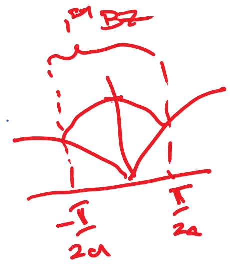
Lecture 17, solid state physics, April 2, 2020

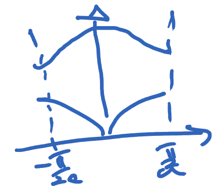
Last time, we considered a 1D chain with a basis

We considered (i) a fake problem by doubling the cell, and (ii) a cell with two different masses and one spring $\mathcal{K}$. You can envision a chain with identical masses and two spring constants: K and G.









lattice $2a$, $b_1 = 0$, $b_2 = a$

The atoms are physically different.

$$V = \sum_L \left[\frac{K}{2}\left(u(2,L) - u(1,L)\right)^2 + \frac{G}{2}\left(u(1,L+1) - u(2,L)\right)^2 \right]$$

↑ potential energy of the system

$$V \to \Theta \to D(k) \Rightarrow \omega_n^2, \hat{e}_n$$

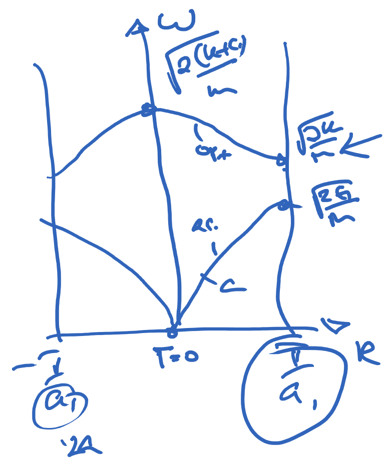
$$\begin{bmatrix} K+G & -K-Ge^{-ika_1} \\ -K-Ge^{ika_1} & K+G \end{bmatrix} \begin{bmatrix} \chi_1^n \\ \chi_2^n \end{bmatrix} = \underline{\underline{M}}\, \omega_n^2(k) \begin{bmatrix} \chi_1^n \\ \chi_2^n \end{bmatrix}$$

$a_1 = 2a$, $n = 1, 2$

$$\omega^2_{n=1/2} = \ldots \pm \ldots$$

$\omega_1^2(k), \hat{e}$

$\chi_i M \chi_j = \delta_{ij}$, $\hat{e}_i \cdot \hat{e}_j = \delta_{ij}$



<u>Long wave limit</u> $k \to 0$ $\left(\frac{2\pi}{k} = \lambda\right)$

$(k=0)$ $\omega_A = 0$, $\omega_0 = \sqrt{\frac{2K+G}{M}}$

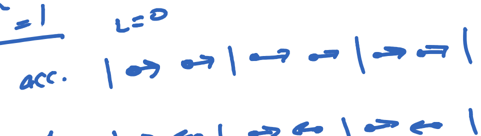
$k \sim 0$ $\sqrt{\frac{KG}{2M(K+G)}}\, ka$ linear dispersion

<u>zone center</u>

(Γ) $\boxed{e_2 = \pm e_1}$ $|e_1|^2 + |e_2|^2 = 1$

↳ a pattern.

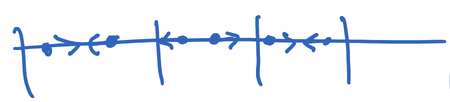
$L = 0$



$\omega(k)$ – the dispersion. $\frac{2\pi}{k} = \lambda$

$(K > G)$ zone edge $k = \frac{\pi}{a_1}$

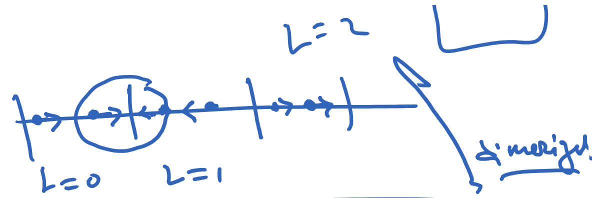
$\omega_0 = \sqrt{\frac{2K}{M}}$ $e_1 = -e_2 \Rightarrow \hat{e}_0 = \begin{pmatrix} \delta \\ -\delta \end{pmatrix}$

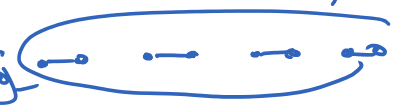


$L = 2$ $e^{i\pi}$

$\omega_{\ldots} = \sqrt{\frac{2G}{\ldots}}$ $e_1 = e_2$ ...

$\omega_a = \sqrt{\frac{2G}{M}}$ $\qquad e_1 = e_2 \Rightarrow \hat{\rho}_a\left(\frac{\pi}{a_1}\right) = \begin{pmatrix} \gamma \\ \gamma \end{pmatrix}$

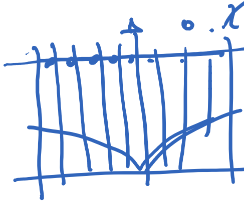




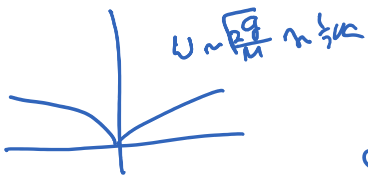
freakish accident of Nature

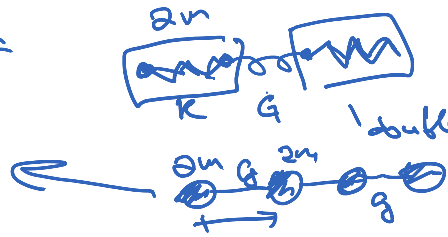
Einstein model

$K \ggg G$
spring constant



ω is independent of $\vec{k}$!
wave vector

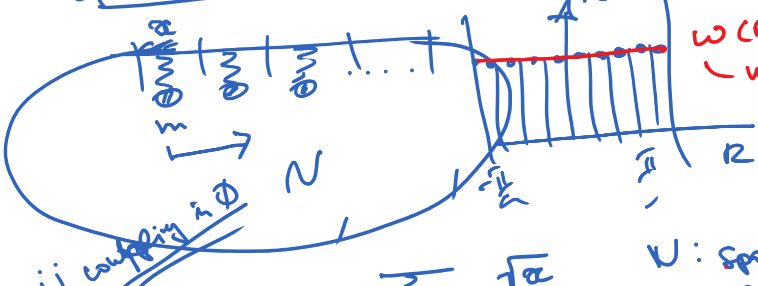


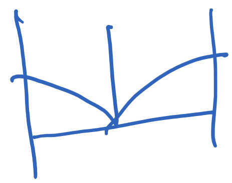


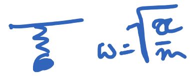
double mass connected by weak spring.

ij coupling!

Einstein's solid

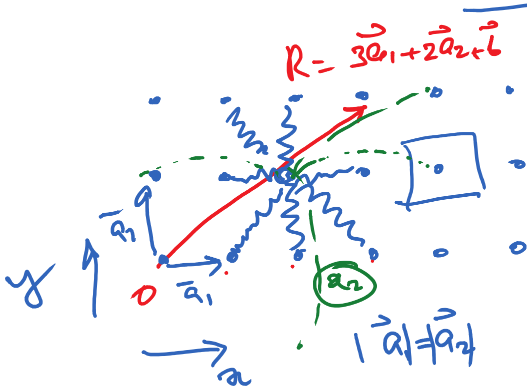






N : spanned by k-values. each with the same frequency.

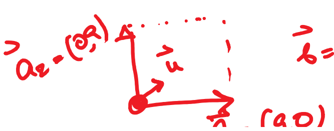
Square lattice



Bravais lattice

$\vec{R}(\ell, m) = \ell\vec{a}_1 + m\vec{a}_2$

one atom per unit cell



$\vec{b} = 0$ – basis

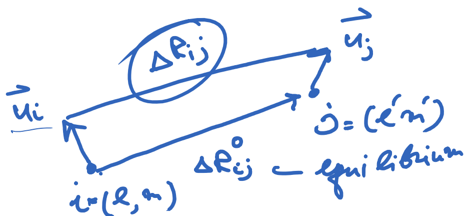
$(a0); (0a)$ – lattice

(harmonic approximation)

I want to set up the small oscillation problem (harmonic approx.)
I want to set up the small oscillation problem regardless of the exact dynamics law.

2×2 problem, regardless of the exact dynamics law.
↳ # of degrees of freedom. $\vec{u}_i = (u_x^i, u_y^i)$

Let's use the "Radial force" approximation.



$\vec{u}_i$ is small compared with $|a|$

at equilibrium, there are no forces!

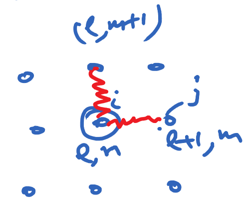
$\frac{\alpha}{2}\left(|\Delta R_{ij}| - |\Delta R^0_{ij}|\right)^2$ ← energy penalty for freedom to move.

$$|\Delta R_{ij}| = \sqrt{\left(R_i^x + u_i^x - R_j^x - u_j^x\right)^2 + \left(R_i^y + u_i^y - R_j^y - u_j^y\right)^2} \simeq$$

$$\simeq \text{easy to show using Taylor expansion} = |\Delta R^0_{ij}|\left(1 + \frac{(\vec{R}_i - \vec{R}_j)\cdot(\vec{u}_i - \vec{u}_j)}{|\Delta R^0_{ij}|^2}\right)$$

$$|\Delta R_{ij}| - |\Delta R^{(0)}_{ij}| \sim \frac{1}{|\Delta R^0_{ij}|}\left(\vec{R}^0_i - \vec{R}^0_j\right)\cdot\left(\vec{u}_i - \vec{u}_j\right)$$

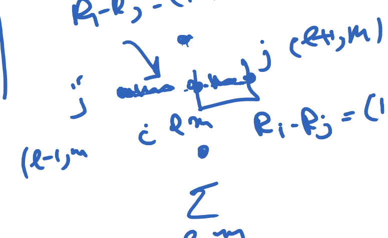
The nearest neighbor approximation.



$|\Delta R^{(0)}_{ij}| = a$

$$(\vec{R}_i - \vec{R}_j) = a\begin{pmatrix}(1\,0)\\(\bar{1}\,0)\\(0\,1)\\(0\,\bar{1})\end{pmatrix}$$

$R_i - R_j = (\bar{1}\,0)$



$R_i - R_j = (1\,0)a$

ΔR^0_{ij} ? a

$\sum_{\ell, m}$

Energy function:
[radial approximation, 1st NN] $(u^x_{\ell m}, u^y_{\ell m}) \to x_{\ell m}, y_{\ell m}$

$x_{\ell m}, y_{\ell m}$: u^x and u^y of atom at (ℓ, m) site.

$$V = \sum\left(\frac{f}{2}\left(x_{\ell+1,m} - x_{\ell,m}\right)^2 + \frac{f}{2}\left(y_{\ell m+1} - y_{\ell m}\right)^2\right)$$

(ℓ, n)

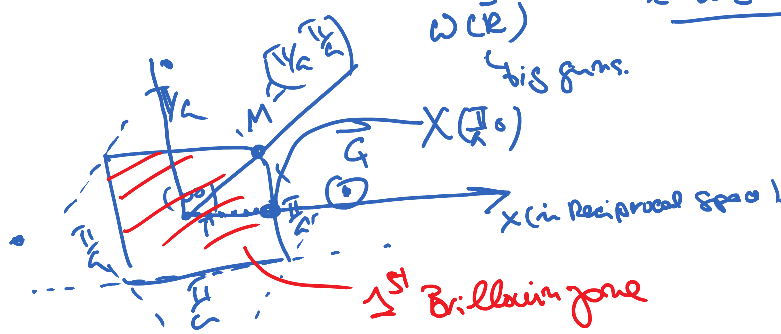
infinite sum over the 2D Bravais lattice.

Θ, $\underline{D}(k) \Rightarrow \omega^2, \hat{e}(\hat{\chi})$

$\frac{\partial V}{\partial x_{\ell n}}, \frac{\partial^2 V}{\partial x_{\ell n} \partial x_{\ell n}} \ldots$

There will be a HW problem on 2D square lattice

k-was a number.



$\cdot (0, -\frac{2\pi}{a})$

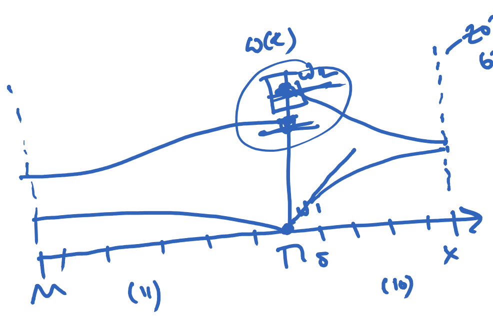
$k_1(00), k_2(0\delta), k_3(0, 2\delta) \ldots$
$\downarrow$
$\underline{D}(k_2)$
ω_1, ω_2

you chose!

$k [0, \frac{\pi}{a}]$: $\vec{k}_1(0,0), \vec{k}_2(\delta, 0), \vec{k}_3(2\delta, 0) \ldots \vec{k}_L(\frac{\pi}{a}, 0)$

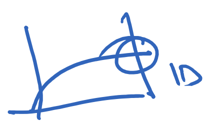
2×2 — $\underline{D}(k_1) \ldots$ $\underline{D}(k_L)$

$\omega_1(k_1)$, $\omega_2(k_1)$ $\quad$ $\omega_1(k_L)$, $\omega_2(k_L)$



$\lim_{k \to \Gamma} \omega \neq \lim_{k' \to \Gamma} \omega$

$|\Gamma M| = \sqrt{2} |\Gamma X|$



$N \to \infty$

We know how to calculate vibrational modes of a crystal

specific heat capacity.

Dulong-Petit 1819 under constant volume $C_v = \frac{3R}{M}$

$R = 8.31 \; J \, K^{-1} mol^{-1}$

molar mass.

$C_{12}H_{22}O_{11}$ $\quad$ $12 \times 12 + 1 \times 22 + 16 \times 11 = 342 \; g/mol$

M – ... (Avogadro) 6.02×10^{23} particles

$$C_V = \left(\frac{\partial E}{\partial T}\right)_V \qquad C_p \text{ (under constant pressure)}.$$

you first need to find the energy E.

$$E = \frac{1}{V}\frac{\int d\Gamma\, e^{-\beta H} H}{\int d\Gamma\, e^{-\beta H}} \qquad \beta = \frac{1}{kT}$$

$$d\Gamma = \prod_{L,\alpha} du_\alpha(L)\, dp_\alpha(L).$$

$$E = -\frac{1}{V}\frac{\partial}{\partial\beta}\ln \underbrace{\int d\Gamma\, e^{-\beta H}}_{\text{the partition function.}} \qquad H \text{ – the Hamiltonian.}$$

$$u = \beta^{-1/2}\tilde{u} \qquad du = \beta^{-1/2} d\tilde{u}$$

$$p = \beta^{-1/2}\tilde{p} \qquad dp = \beta^{-1/2} d\tilde{p}$$

$$\boxed{H = \sum \frac{p^2}{2m} + U_{eq} + U_{harm}} \quad U_{harm} = \sum_{\substack{LL'\\ \alpha\alpha'}} u\Theta u$$

$$\int \underbrace{\prod du\, dp}_{d\Gamma} \exp\left(-\beta\left(\sum\frac{p^2}{2m} + U_{eq} + \frac{1}{2}\sum \Theta u u\right)\right) =$$

$$= \int e^{-\beta U_{eq}} \prod \beta^{-1} d\tilde{u}\, d\tilde{p}\, \exp\left[-\beta^{-1}\sum\frac{\tilde{p}^2}{2m} - \frac{1}{2}\beta^{-1}\sum\Theta u u\right] =$$

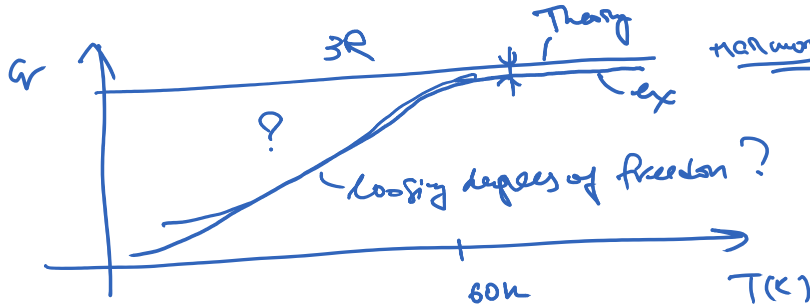
$$= e^{-\beta U_{eq}} \beta^{-3N} \underbrace{\left\{\int\prod d\tilde{u}\, d\tilde{p}\, \exp\left[-\sum\frac{\tilde{p}^2}{2m} - \frac{1}{2}\sum\tilde{u}\Theta\tilde{u}\right]\right.}_{\text{independent of } \beta}$$

$$E = -\frac{1}{V}\frac{\partial}{\partial\beta}\ln\left(e^{-\beta U_{eq}}\beta^{-3N} \times \text{const}\right) = \frac{U^{eq}}{V} + \frac{3N}{V}kT$$

$E = -\frac{1}{V}\frac{\partial}{\partial\beta}$ ...

$C_V = \frac{\partial E}{\partial T} = \frac{3N}{V} k$

$kN = R$ for a mole. Dulong-Petit



harmonic approx

Equipartition: $\frac{1}{2}kT$ / deg. of freed. Low T experiments killed it.

$\frac{6N}{2}kT$

you have to go Quantum!!!