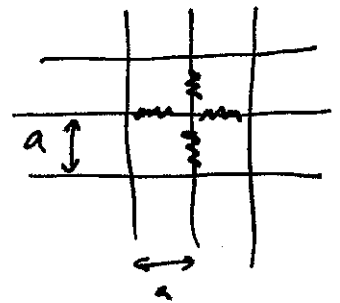


Solutions to homework set III

①

Square lattice with nearest neighbor

interactions of the form $\frac{1}{2} k (r_{ij} - a)^2$



$\vec{r}_{ij} = \vec{R}_i + \vec{u}_i$ → displacement from equilibrium ($u \ll a$)
 ↙ equilibrium position

$$r_{ij} = |\vec{R}_{ij} + \vec{u}_{ij}| = \sqrt{(R_{ij}^x + u_{ij}^x)^2 + (R_{ij}^y + u_{ij}^y)^2}$$

Clearly this is not a polynomial in u , so we have to expand it in powers of u and take the second order terms.

$$r_{ij} = \sqrt{a^2 + 2a u_{ij}^x + (u_{ij}^x)^2 + (u_{ij}^y)^2}$$

since $\begin{cases} R_{ij}^x = 0 \text{ or } a \\ R_{ij}^y = a \text{ or } 0 \end{cases}$

$$= a \left[1 + \frac{2a u_{ij}^x}{a^2} + \frac{(u_{ij}^x)^2 + (u_{ij}^y)^2}{a^2} \right]^{\frac{1}{2}} \rightarrow \text{for } \begin{cases} R_{ij}^x = a \\ R_{ij}^y = 0 \end{cases} \text{ for example.}$$

$$\cong a \left[1 + \frac{u_{ij}^x}{a} + \mathcal{O}(u^2) \right]$$

$$V^H = \frac{K}{2} \sum_{\langle ij \rangle} 2(u_{ij}^x)^2 + 2(u_{ij}^y)^2$$

(factors of 2 come from the 2 neighbors at $(-a, 0)$ and $(0, a)$ or $(0, a)$ and $(0, -a)$)

$$F_{ix} = - \frac{\partial V^H}{\partial u_i^x} = - \sum_{j=1}^2 2K (u_i^x - u_j^x)$$

($\alpha = x \text{ or } y$) → F_x only comes from $(a, 0)$ & $(-a, 0)$ neighbors

$$M \frac{d^2 u_i^\alpha}{dt^2} = F_{ix} = -2K \sum_{j=1}^2 (u_i^\alpha - u_j^\alpha)$$

j refers to the 2 neighbors

Note the way the potential was defined, the spring constant between a pair turns out to be $2K$ in this case.

Using $\vec{u}_k(t) = \sum_i \vec{u}_i e^{i(kR_i - \omega t)}$

$$M \frac{d^2 u_i^x}{dt^2} = -2K \sum_{j=1}^2 (u_i^x - u_j^x) = -2K (u_i^x - u_{i+a\hat{x}}^x - u_{i-a\hat{x}}^x)$$

$$M \frac{d^2 u_i^y}{dt^2} = -2K (2u_i^y - u_{i+a\hat{y}}^y - u_{i-a\hat{y}}^y)$$

multiply by e^{ikR_i} and sum over i

$$-M\omega^2 u_k^x = -2K [u_k^x - u_k^x (e^{-ik_x a} + e^{ik_x a})]$$

$$-M\omega^2 u_k^y = -2K [2u_k^y - u_k^y (e^{-ik_y a} + e^{ik_y a})]$$

Now the equations are decoupled in u_k and we have N independent harmonic oscillators for which the dynamical matrix is diagonal:

Diagonal elements are: $\begin{cases} -M\omega^2 + 2K(2 - 2\cos k_x a) \\ -M\omega^2 + 2K(2 - 2\cos k_y a) \end{cases}$
 off-diagonal elements are: 0.

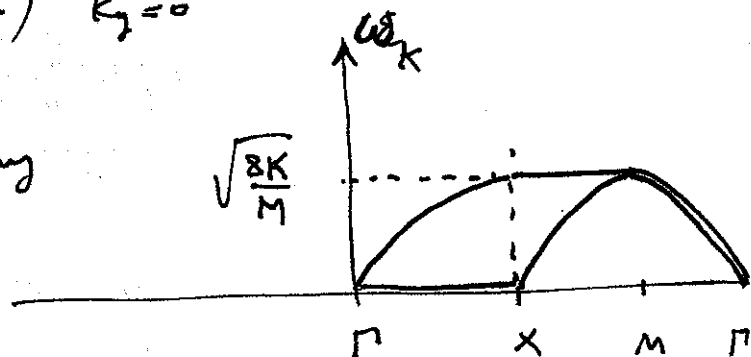
$$\omega_x^2 = \frac{4K}{M} (2 - \cos k_x a) = \frac{8K}{M} \sin^2 \frac{k_x a}{2}$$

$$\omega_y^2 = \frac{4K}{M} (1 - \cos k_y a) = \frac{8K}{M} \sin^2 \frac{k_y a}{2}$$

if $\vec{k} = (k, 0)$ (along \hat{x}) $k_y = 0$

$\omega_x \neq 0$ but $\omega_y = 0$

this "transverse" mode is very "soft" causing the crystal to become unstable.



If you go back to the original potential you'll see that it does not take ANY energy to

fold the bond angles. (since 2nd neighbors are neglected)

So we have 2 branches (1 atom/unit cell) in 2D

Along X or Y directions however one branch is zero, due to the neglect of 2nd neighbor interactions, causing this instability.

Debye model: replace $\sqrt{\frac{8K}{M}} \sin \frac{k_x a}{2}$ by $c_x k_x$ & $c_y k_y$
where $c =$ speed of sound (longitudinal & transverse)

We see that the speeds of sound depend on the direction

of propagation (\hat{k})

$$c_l(k\hat{x}) = \frac{a}{2} \sqrt{\frac{8K}{M}} \quad \left(\frac{\partial \omega_x}{\partial k_x} \right)$$

$$c_t(k\hat{x}) = 0$$

$$\frac{\partial}{\partial k} = \frac{\partial}{\partial k_x} \frac{\partial k_x}{\partial k} + \frac{\partial}{\partial k_y} \frac{\partial k_y}{\partial k}$$

$$k_x = k \cos \theta$$

$$\frac{\partial k_x}{\partial k} = \cos \theta$$

$$k_y = k \sin \theta$$

$$\frac{\partial k_y}{\partial k} = \sin \theta$$

$$c_1 = \frac{\partial}{\partial k} \left(\omega_0 \sin \frac{k_x a}{2} \right) = \omega_0 \frac{a}{2} \cos \frac{k_x a}{2} \times \cos \theta$$

$$\xrightarrow{k \rightarrow 0} \frac{a}{2} \cos \theta \times \sqrt{\frac{8K}{M}}$$

$$c_2 = \frac{\partial}{\partial k} \left(\omega_0 \sin \frac{k_y a}{2} \right) \xrightarrow{k \rightarrow 0} \frac{a}{2} \sin \theta \sqrt{\frac{8K}{M}}$$

$$\downarrow \omega_0$$

$$\Rightarrow c_l = \omega_0 \frac{a}{2} \times \text{Max}(\cos \theta, \sin \theta)$$

$$c_t = \omega_0 \frac{a}{2} \times \text{Min}(\cos \theta, \sin \theta)$$

This is unusual since in

the $k \rightarrow 0$ limit $c = \left. \frac{\partial \omega}{\partial k} \right|_{k \rightarrow 0}$ is independent of k & its direction.

$$\omega_D \text{ is defined by } Nk^2 = \int_0^{\omega_D} \text{dos}(\omega) d\omega$$

$$\text{in 2D } \text{dos}(\omega) d\omega = \text{dos}(k) dk = \frac{2\pi k dk}{\left(\frac{2\pi}{L}\right)^2} \rightarrow \text{assumes isotropy in } \omega(k)$$

$$\text{assuming } \omega = ck \quad \text{dos}(\omega) = \frac{1}{c^2} \times \frac{L^2}{2\pi} \times \omega$$

so for c we take the angular average of c_l, c_t .

$$C_e = C_t = \frac{\omega_0 a}{2} \langle |\cos \theta| \rangle = \frac{\omega_0 a}{2} \int_0^{2\pi} |\cos \theta| \frac{d\theta}{2\pi} = \frac{\omega_0 a}{2} \cdot \int_0^{\pi/2} \cos \theta \frac{d\theta}{(\pi/2)}$$

$$= \frac{\omega_0 a}{2} \cdot \frac{2}{\pi} = \frac{\omega_0 a}{\pi}$$

$$\Rightarrow \text{DOS}(\omega) = \frac{L^2}{2\pi} \frac{\pi^2}{\omega_0^2 a^2} \times 2 \times \omega$$

↳ 2 Modes (l and t)

$$N \times 2 = \int_0^{\omega_D} \frac{L^2 \pi}{\omega_0^2 a^2} \omega d\omega = \frac{L^2 \pi}{\omega_0^2 a^2} \frac{\omega_D^2}{2}$$

but $\frac{L^2}{a^2} = N \Rightarrow \boxed{\omega_D = 2\omega_0 / \sqrt{\pi}}$ with $\omega_0 = \sqrt{\frac{8K}{M}}$

So that $\frac{\text{DOS}(\omega)}{N} = \text{dos per cell} = \frac{\pi \omega}{\omega_0^2} = \frac{4\omega}{\omega_D^2}$

$$C_v / \text{cell} = \int_0^{\omega_D} \left[\frac{\beta \hbar \omega / 2}{\sinh \frac{\beta \hbar \omega}{2}} \right]^2 \times k_B \text{ dos}(\omega) d\omega = k_B \int \left(\frac{x}{\sinh x} \right)^2 \frac{4}{\omega_D^2} \left(\frac{2}{\beta \hbar} \right)^2 x dx$$

Summation
heat capacity per mode
of modes

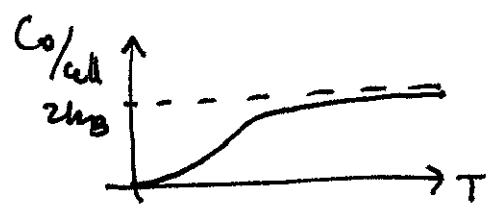
$$C_v / \text{cell} = \frac{16 k_B}{(\beta \hbar \omega_D)^2} \int_0^{\beta \hbar \omega_D / 2} \frac{x^3}{(\sinh x)^2} dx$$

* high T $\beta \hbar \omega_D \rightarrow 0 \quad \left(\frac{x}{\sinh x} \right)^2 \rightarrow 1. \quad C_v = \frac{16 k_B}{(\beta \hbar \omega_D)^2} \frac{1}{2} (\beta \hbar \omega_D)^2 = 2k_B$

expected classical result in 2D with one atom/cell

* low T $\beta \hbar \omega_D \rightarrow \infty$

$$C_v / \text{cell} \approx \frac{16 k_B}{(\beta \hbar \omega_D)^2} \int_0^{\infty} \frac{x^3}{(\sinh x)^2} dx \propto T^2$$

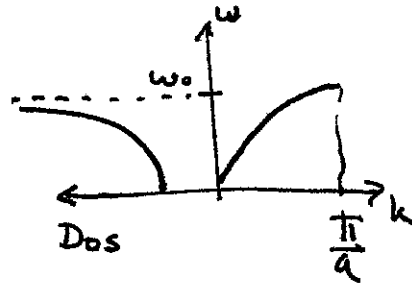


This is true, unlike this simplified model for a stable 2D solid with isotropic dispersion at small k

1 - Singularity in DOS

Dispersion relation obtained was: $\omega(k) = \omega_0 \sinh\left(\frac{ka}{2}\right)$.

$$\omega_0 = \sqrt{\frac{4C}{M}}$$



a) In 1D, Dos is defined by $(k \& -k)$

$$DOS(\omega) d\omega = 2 \times \frac{L}{2\pi} \times dk$$

$$\frac{d\omega}{dk} = \omega_0 \frac{a}{2} \cosh\left(\frac{ka}{2}\right) = \frac{\omega_0 a}{2} \sqrt{1 - \frac{\omega^2}{\omega_0^2}}$$

$$\Rightarrow D(\omega) = \frac{L}{\pi} \frac{2}{\omega_0 a} \frac{1}{\sqrt{1 - \frac{\omega^2}{\omega_0^2}}} = \frac{2N}{\pi} \frac{1}{\sqrt{\omega_0^2 - \omega^2}} \quad \left(N = \frac{L}{a}\right)$$

b) $\omega(k) = \omega_0 - Ak^2$ in 3D, ($A > 0$)

$$D(\omega) d\omega = \left(\frac{L}{2\pi}\right)^3 4\pi k^2 dk \quad \frac{d\omega}{dk} = -2Ak$$

$$\Rightarrow D(\omega) = \left(\frac{L}{2\pi}\right)^3 \frac{4\pi}{+2A} \left(\frac{\omega_0 - \omega}{A}\right)^{1/2} \quad \text{for } \omega < \omega_0 \quad \left|\frac{d\omega}{dk}\right| = +2A \sqrt{\frac{\omega_0 - \omega}{A}}$$

& of course since there are no states above ω_0 , $D(\omega) = 0$ for $\omega > \omega_0$.

Kittel chap 6 pb 1.

Kinetic energy of 3D free electrons at $T=0$

$$T = \sum_{k \in \text{occ}} \frac{\hbar^2 k^2}{2m} = \int_0^{\mu} DOS(E) E dE = \frac{V}{(2\pi)^2} \left(\frac{2m}{\hbar^2}\right)^{3/2} \mu^{5/2} \times \frac{2}{5}$$

But $N = \sum_{k \in \text{occ}} 1 = \int_0^{\mu} DOS(E) dE$ relates μ to N ($\mu = E_F$)

$$N = \frac{V}{(2\pi)^2} \left(\frac{2m}{\hbar^2}\right)^{3/2} \mu^{3/2} \times \frac{2}{3} \Rightarrow \frac{T}{N} = \frac{2}{5} \frac{\mu}{\frac{2}{3}} = \frac{3\mu}{5} \Rightarrow T = \frac{3}{5} N E_F$$

Pressure & Bulk modulus of an electron gas.

For a free electron gas, the total energy is just the kinetic energy $E_0 = \frac{3}{5} N E_F$ this gives you the equation of state at $(T=0)$

a) $P = -\left(\frac{\partial E_0}{\partial V}\right)_N$; $E_F = \mu$ is related to N through $N = A \mu^{3/2}$
(or $n = \frac{k_F^3}{3\pi^2}$)

$$\left(\frac{\partial E_0}{\partial V}\right)_N = \left(\frac{\partial E_0}{\partial n}\right) \left(\frac{\partial n}{\partial V}\right)_N = \frac{3}{5} N \cdot \frac{\partial \mu}{\partial n} \times \left(-\frac{N}{V^2}\right)$$

$$\begin{aligned} \frac{\partial \mu}{\partial n} &= \frac{\partial \left(\frac{\hbar^2 k_F^2}{2m}\right)}{\partial n} = \frac{\hbar^2}{2m} \frac{\partial (3\pi^2 n)^{2/3}}{\partial n} = \frac{\hbar^2}{2m} (3\pi^2)^{2/3} \frac{2}{3} n^{-1/3} \\ &= \frac{\hbar^2}{2m} \frac{2}{3} (3\pi^2)^{2/3} \cdot \frac{1}{k_F} = \frac{2}{3} \frac{\mu}{n} \quad (\text{Also in general } \frac{\partial \mu}{\partial n} = \frac{1}{\text{DOS}}) \end{aligned}$$

$$\Rightarrow P = \frac{3}{5} n^2 \times \frac{2}{3} \frac{\mu}{n} = \frac{2}{5} n \mu = \frac{2}{5} n \times \frac{5}{3} \frac{E_0}{N} = \boxed{\frac{2}{3} \frac{E_0}{V} = P}$$

b) $B = -V \left(\frac{\partial P}{\partial V}\right)_N = -\left(\frac{\partial P}{\partial \ln V}\right)_N$; $V = \frac{N}{n}$; $\ln V = \ln N - \ln n$

$$= + \left(\frac{\partial P}{\partial \ln n}\right) \quad P = \frac{2}{3} \frac{E_0}{V} = \frac{2}{3} \frac{3}{5} \frac{N}{V} E_F = \frac{2}{5} n \cdot (3\pi^2 n)^{2/3} \frac{\hbar^2}{2m}$$

$$\Rightarrow P \propto n^{5/3} \quad \Rightarrow n \frac{\partial P}{\partial n} = \frac{5}{3} n^{2/3} \times n = \boxed{\frac{5}{3} P = B}$$

c) for K : $n = 1.4 \cdot 10^{28} \text{ e/m}^3$; $k_F = 0.75 \text{ \AA}^{-1} \times 10^8$; $E_F = 2.12 \text{ eV}$

$$\begin{aligned} \frac{E_0}{V} &= \frac{3}{5} n E_F \Rightarrow P = \frac{2}{5} n \frac{\hbar^2}{2m} k_F^2 = 0.4 \times 1.4 \cdot 10^{28} \cdot 2.12 \cdot 1.6 \cdot 10^{-19} \\ &= 1.9 \cdot 10^9 \text{ Pa} \quad \Rightarrow B = \frac{5}{3} P = 3.16 \cdot 10^9 \text{ Pa} \end{aligned}$$

Kittel Chap 6, Pb 3.

chemical potential in 2D ...

... is obtained from expressing the e^- density as:

$$n_{2D} = \int_0^{\infty} \text{dos}(E) f(E) dE$$

where $\text{dos}(E)$ is the DOS per unit volume

$$\text{in 2D } \text{dos}(E) dE = \frac{1}{(2D)^2} \times 2 \times 2\pi k dk \quad dE = \frac{\hbar^2}{m} k dk$$

↳ spin

$$\Rightarrow \text{dos}(E) = \frac{m}{\pi \hbar^2} \quad (= \text{constant}) \quad \text{per unit volume.}$$

$$n = \frac{m}{\pi \hbar^2} \int_0^{\infty} f(E) dE \quad ; \quad \int_0^{\infty} \frac{dE}{1 + e^{\beta(E-\mu)}} = \int_0^{\infty} \frac{e^{-\beta(E-\mu)}}{e^{-\beta(E-\mu)} + 1} dE = \frac{1}{\beta} \ln(1 + e^{\beta\mu})$$

$$\Rightarrow \ln(1 + e^{\beta\mu}) = \frac{\beta n}{\text{dos}} \Rightarrow \mu = kT \ln\left(e^{\frac{\beta n}{\text{dos}}} - 1\right)$$

$$\text{or } \mu = k_B T \ln\left(e^{\frac{\pi \hbar^2 n}{m k_B T}} - 1\right)$$