3. Fermi Gas. — Non interacting fermions + exclusion

$$-\frac{\hbar^2}{2m}\nabla^2\psi = E\psi \rightarrow \psi_k = e^{i\underline{k}.\underline{r}}$$

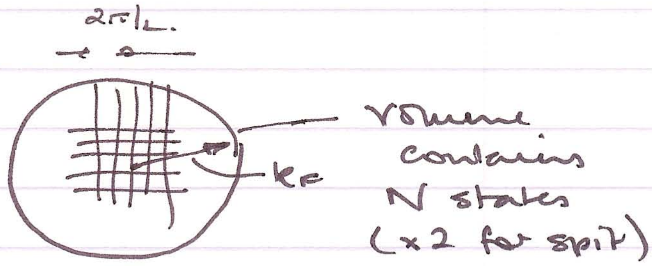
$$E_k = \frac{\hbar^2 k^2}{2m} \quad (+\ \sigma = \uparrow\downarrow).$$

Periodic Boundary conditions on box (L, L, L)

$$\psi_k(x+L, y, z) = \psi_k(x, y, z) \Rightarrow e^{ik_x L} = 1$$

$$k = \frac{2\pi}{L}(n_x, n_y, n_z) \qquad n_x = 0, \pm 1, \pm 2, \ldots \text{ etc.}$$

- Density of states:



$$N = 2\frac{\left(\frac{4\pi}{3}k_F^3\right)}{(2\pi/L)^3} \Rightarrow N = V.\frac{8\pi}{3.}\frac{k_F^3}{8\pi^3}$$

$$\Rightarrow k_F = \left(3\pi^2\frac{N}{V}\right)^{1/3}.$$

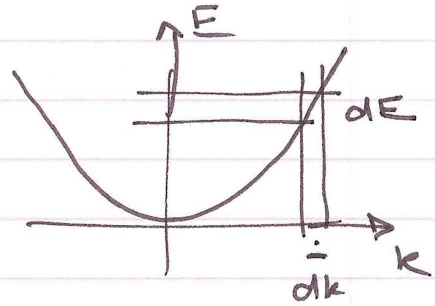
$$E_F = \frac{\hbar^2 k_F^2}{2m}$$

- Sums and integrals.

$$\sum_{\underline{k}} f(|k|) \simeq \underset{\text{spin}}{2}\left(\frac{L}{2\pi}\right)^3 \int d^3k\, f(k) = \frac{2V}{(2\pi)^3}\int dk\, k^2.4\pi f(k)$$

$$= \frac{V}{\pi^2}\int dk.k^2 f(k)$$

Density of states in energy.



$$g(E)\,dE = 2.\frac{\text{Vol of shell}}{\text{Vol of k-space/state.}}$$

$$= 2.\frac{4\pi k^2 dk}{(2\pi)^3/V}$$

$$g(E) = \frac{V}{\pi^2}k^2\frac{dk}{dE} = \frac{V}{\pi^2}\frac{m}{\hbar^2}\left(\frac{2mE}{\hbar^2}\right)^{1/2}.$$

- Thermal properties.

Occupancy : Fermi function $f(E) = \dfrac{1}{e^{\beta(E-\mu)}+1}$

$\beta = 1/k_BT$.

<u>Density</u> : $n = \dfrac{N}{V} = \dfrac{2}{V}\sum_k f(E_k) = \int dE\, g(E) f(E)$

→ determines μ

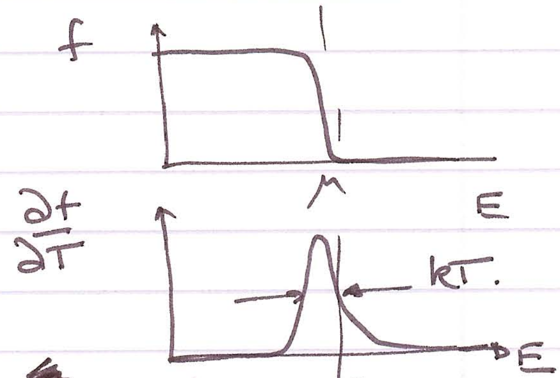
Internal <u>energy</u> : $u = \dfrac{U}{V} = \int dE . E\, g(E) f(E)$

Specific heat.

$$C_V = \int dE.\, E. g(E) \frac{\partial f(E)}{\partial T}.$$

Remember : $\mu \gg k_BT$.

⇒ Contribution <u>only</u> from states near μ



Classical gas: $C_V = n . \frac{3}{2} k_B$. at large T

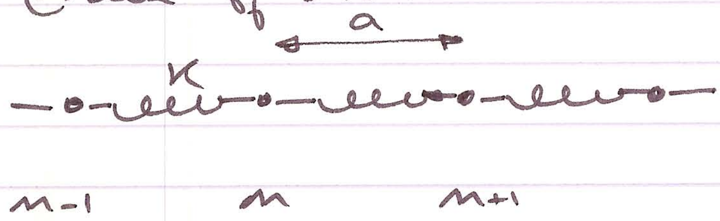
Fermi gas: $C_V = n . \frac{\pi^2}{2} k_B \left(\dfrac{k_BT}{\mu}\right)$ $\mu \sim E_F$

Notes —— also. show $\mu = E_F \left[1 - \frac{1}{3}\left(\frac{\pi}{2}\frac{k_BT}{E_F}\right)^2 + \dots \right]$

<u>small</u>

Lattice Dynamics:

1D Chain of atoms.



Equ^{m} small.

$u = \underset{r_n}{na} + u_n(t)$

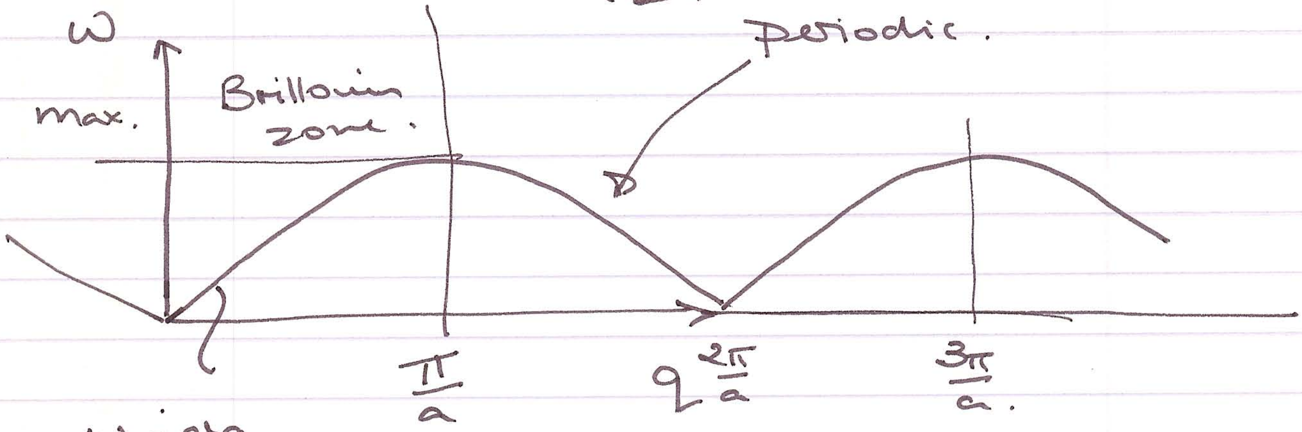
Equ^{n} of motion

$$m\ddot{u}_n = K(u_{n+1}-u_n) + K(u_n-u_{n-1}) \quad (1)$$

Solution: $u_n(t) = u_0 e^{i(qr_n - \omega t)}$.

⇒ substitute in (1), simplify.

⇒ $m\omega(q)^2 = 4K\sin^2\left(\frac{qa}{2}\right)$ — dispersion relation

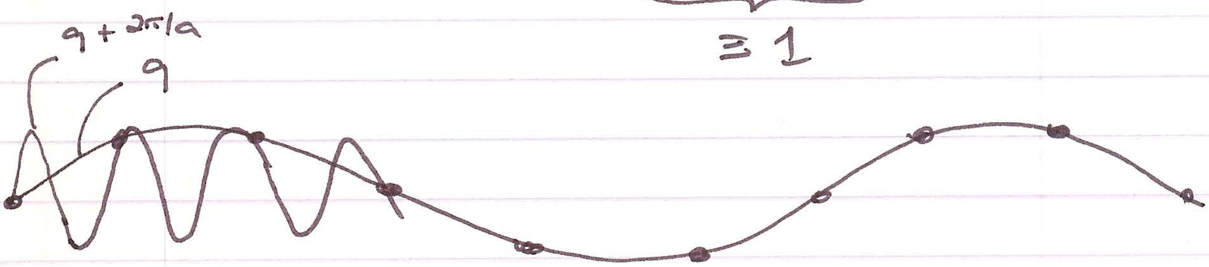


$\omega \doteq vq$

$v = \left(\frac{Ka^2}{m}\right)^{1/2}$ — sound velocity

N.B. $q \rightarrow q + \frac{2\pi}{a}$.

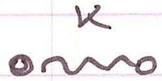
$$u_n = u_0 e^{i(qr_n - \omega t)} \underbrace{e^{i\frac{2\pi}{a}na}}_{\equiv 1}$$



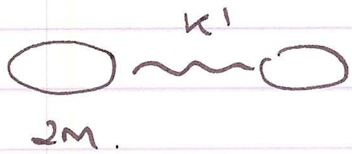
Diatomic chain:

Simplified case $K \gg K'$ and $m_A = m_B$.

Dimer.



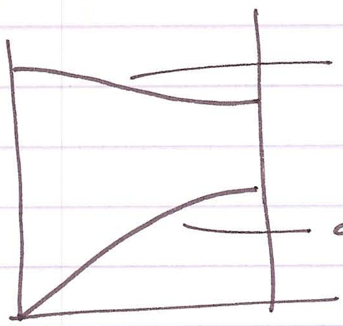
$\Rightarrow \omega_0^2 = \frac{2K}{m}$. (indep of q)



$\Rightarrow$ acoustic mode.

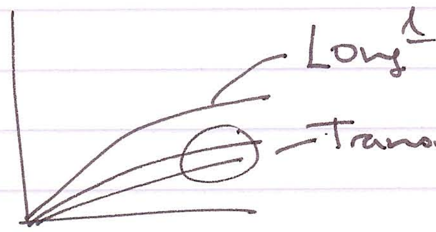
$\omega^2 = \left(\frac{K'}{2m}\right) \sin^2\left(\frac{qa}{2}\right)$

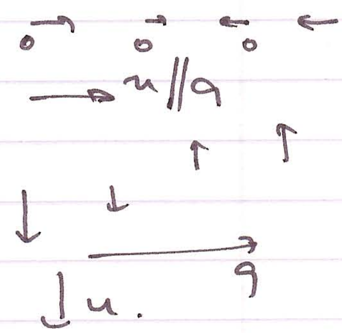
Prob 3.6



(sometimes visible by absorbing / scattering light).

3D solids $\rightarrow$ 3D dispersion $\omega(\vec{k})$.





m atoms / cell

$\rightarrow$ 3 acoustic

3(m-1) optic modes.

P.B.C $\quad k_n = \frac{2\pi}{L}(n_x, n_y, n_z)$

Now $-\frac{N}{2}, \ldots \leq n < \frac{N}{2}$

so $-\frac{\pi}{a} < k < \frac{\pi}{a}$:

Total no of states $= 3.m.N$ ✓

Density of States — Einstein & Debye Models

Einstein — $D(\omega) = N\,\delta(\omega-\omega_0)$ ← # of atoms.

Eqn. (3.43)
3.43 error

Debye. — $D(\omega) = \dfrac{4\pi k^2}{(2\pi/L)^3}\underbrace{\dfrac{dk}{d\omega}}_{\omega = vk.} = \dfrac{V\omega^2}{2\pi^2 v^3}$

— needs a cutoff.

$$N = \int_0^{\omega_D} D(\omega)\,d\omega = \frac{V}{v^3}\,\frac{1}{2\pi^2}\,\frac{1}{3}\,\omega_D^3.$$

(3.46) $V \to v$

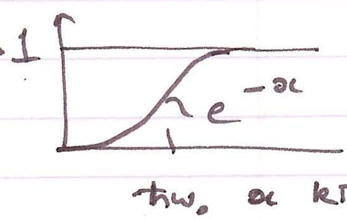
Lattice thermal prop.

Occ. $n(\omega) = \dfrac{1}{e^{\beta\omega}-1}$: $\mu = 0$, N_{ph} not conserved.

$$U = \int d\omega\, D(\omega)\, n(\omega) . \hbar\omega .$$

$$U_E = N . \hbar\omega_0 . \frac{1}{e^{\hbar\omega_0/kT}-1}$$

$$= N . k_B T . \left[\frac{x}{e^x - 1}\right] \quad \text{where } x = \frac{\hbar\omega_0}{kT}$$



Eqn. (3.51) v^3

$$U_D = \int_0^{\omega_D} d\omega\, \frac{V\omega^2}{2\pi^2 v^3}\, \frac{\hbar\omega}{e^{\hbar\omega/kT}-1} \quad \sim \quad x = \hbar\omega/kT$$

$$= \frac{V}{2\pi^2 v^3}\left(\frac{kT}{\hbar}\right)^4 \hbar \int_0^{\frac{\hbar\omega_D}{kT}} \frac{dx\, x^3}{(e^x - 1)}$$

$$= 3N(kT)\left(\frac{kT}{\hbar\omega_D}\right)^3 \int_0^{\frac{\hbar\omega_D}{kT}} \frac{dx\, x^3}{(e^x-1)}$$

→ $C_V \propto T^3$ at low T.