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Assignment - 2

Q.2) Show that

$$\int_0^\infty \frac{\eta^j}{e^\eta + 1}\, d\eta = \Gamma(j+1)\left(1 - 2^{-j}\right)\zeta(j+1)$$

where, Riemann Zeta Function is given by,

$$\zeta(s) = \sum_{n=1}^{\infty} \frac{1}{n^s}$$

Ans

$$\int_0^\infty d\eta\, \frac{\eta^j}{e^\eta + 1} = \int_0^\infty d\eta\, \frac{\eta^j e^{-\eta}}{1 + e^{-\eta}}.$$

Now see

$$e^{-\eta} - e^{-2\eta} + e^{-3\eta} - \cdots = \frac{e^{-\eta}}{1 + e^{-\eta}} = \sum_{m=1}^{\infty} e^{-m\eta}(-1)^{m+1}$$

$\therefore$ LHS

$$= \int_0^\infty d\eta\, \eta^j \sum_{m=1}^{\infty} e^{-m\eta}(-1)^{m+1}$$

make a substitution, $m\eta = u \quad d\eta = \frac{du}{m}$

$$\therefore = \sum_{m=1}^{\infty} \frac{(-1)^{m+1}}{m^{j+1}} \underbrace{\int_0^\infty u^j e^{-u}\, du}_{= \Gamma(j+1)}$$

Now, we have to manipulate the sum.

$$\sum_{m=1}^{\infty} \frac{(-1)^{m+1}}{m^{j+1}} = \frac{1}{1} - \frac{1}{2^{j+1}} + \frac{1}{3^{j+1}} - \frac{1}{4^{j+1}} \cdots$$

$$= \left(1 + \frac{1}{2^{j+1}} + \frac{1}{3^{j+1}} + \frac{1}{4^{j+1}} + \cdots\right)$$

$$-2\left(\frac{1}{2^{j+1}} + \frac{1}{4^{j+1}} + \frac{1}{6^{j+1}} + \cdots\right)$$

$$= \left(1 - \frac{1}{2^{j+1}}\right)\left(1 + \frac{1}{2^{j+1}} + \frac{1}{3^{j+1}} + \frac{1}{4^{j+1}} + \cdots\right)$$

$$= (1 - 2^{-j})\,(\zeta(j+1))$$

Hence,

$$\int_0^\infty \eta^j \frac{d\eta}{e^\eta + 1} = \Gamma(j+1)\,(1-2^{-j})\,\zeta(j+1).$$

D

Q. 7) $T \ll T_F \therefore \beta\mu \gg 1$

Start from.

$$I = \int_0^\infty H(E) \frac{1}{e^{(E-\mu)/k_B T} + 1} dE,$$

where $H(E) = E^\nu$, which vanishes at $E = 0$. Using the saddle-point approximation, derive

$$I \triangleq \int_0^\mu H(E)\,dE + \frac{\pi^2}{6}(k_B T)^2 H'(\mu) + \mathcal{O}(T^4)$$

Now, let $\boxed{x = \beta E}$ $\therefore dE = \frac{dx}{\beta}$.

$$\therefore I = \frac{1}{\beta} \int_0^\infty H(x/\beta) \frac{dx}{e^x z^{-1} + 1}$$

Now,
$H(E) = E^\nu$
$\therefore H\left(\frac{x}{\beta}\right) = \left(\frac{x}{\beta}\right)^\nu$

Let

$$\therefore I \equiv F_\nu(z) = \frac{1}{\beta^{\nu+1}} \int_0^\infty \frac{x^\nu\,dx}{z^{-1}e^x + 1}$$

We would now like to do the large-z-expansion of $F_\nu(z)$.
Break the integrand!

$$I = \frac{1}{\beta^{\nu+1}}\left[\int_0^{\beta\mu} dx \frac{x^\nu}{z^{-1}e^x + 1} + \int_{\beta\mu}^\infty dx \frac{x^\nu}{z^{-1}e^x + 1}\right]$$

$$\beta^{\nu+1} I = \int_0^{\beta\mu} dx\, x^{\nu}\left[1 - \frac{1}{1+z e^{-x}}\right] + \int_{\beta\mu}^{\infty} dx\, \frac{x^{\nu}}{z^{-1}e^{x}+1}$$

Pg-2

$$= \int_0^{\beta\mu} dx\, x^{\nu} - \int_0^{\beta\mu} dx\, \frac{x^{\nu}}{z e^{-x}+1} + \int_{\beta\mu}^{\infty} dx\, \frac{x^{\nu}}{z^{-1}e^{x}+1}$$

Subst. $\eta_1 = \beta\mu - x$

Subst. $\eta_2 = x - \beta\mu$

Since $T \ll T_F$

$\therefore \beta\mu \gg 1$

~~Firstly we note that the first integral~~

$$= \int_0^{\beta\mu} dx\, x^{\nu} - \int_0^{\beta\mu} d\eta_1 \frac{(\beta\mu-\eta_1)^{\nu}}{z^{-1}+e^{\eta_1}} + \int_0^{\infty} d\eta_2 \frac{(\beta\mu+\eta_2)^{\nu}}{1+e^{\eta_2}}$$

Firstly, we note that first integral has e^{η_1} suppression in the denominator. If we replace the upper limit of the integral by ∞, the expression changes by a term of order $e^{-\beta\mu} = z^{-1} \rightsquigarrow$ which we want to neglect. With this approximation we can combine the two integrals into one.

2nd term

$$\simeq \int_0^{\infty} d\eta \frac{(\beta\mu+\eta)^{\nu} - (\beta\mu-\eta)^{\nu}}{1+e^{\eta}}$$

Taylor expanding Numerator.

$$= (\beta\mu)^{\nu}\left[(1+\eta/\beta\mu)^{\nu} - (1-\eta/\beta\mu)^{\nu}\right]$$

$$= (\beta\mu)^{\nu}\left[1 + \nu\frac{\eta}{\beta\mu} + \cdots - 1 + \nu\frac{\eta}{\beta\mu} + \cdots\right]$$

$$= 2\nu\,(\beta\mu)^{\nu-1}\eta + \cdots \mathcal{O}((\beta\mu)^{\nu-2})$$

$\therefore$ 2nd term $\simeq 2\nu\,(\beta\nu)^{\nu-1} \int_0^{\infty} d\eta \frac{\eta}{1+e^{\eta}}$

Thus putting $j = 1$, in Formula in Q2)

$$\int_0^\infty dy \frac{\eta}{e^\eta + 1} = \Gamma(2) \left(1 - \frac{1}{2}\right) \zeta(2)$$

$$= 1 \times \frac{1}{2} \times \frac{\pi^2}{6}$$

$$\therefore \beta^{\nu+1} I \simeq \int_0^{\beta\mu} dx\, x^\nu + \chi\nu\, \beta^{\nu-1} \mu^{\nu-1} \frac{1}{\chi} \frac{\pi^2}{6}$$

$$I \simeq \int_0^{\beta\mu} \frac{dx}{\beta} \left(\frac{x}{\beta}\right)^\nu + \beta^{-2} (H'(\mu)) \frac{\pi^2}{6}$$

Subst. back $E = \frac{x}{\beta}$

$$I \simeq \int_0^{\mu} H(E)\, dE + \frac{\pi^2}{6} (K_B T)^2 H'(\mu) + \mathcal{O}(T^4)$$

□

Q6) A classical paramagnetic material consists of N non-interacting magnetic dipoles of magnitude μ at thermal equilibrium in a uniform external magnetic field induction B at temp. T.

Find partition function, Magnetisation M and magnetic susceptibility $\chi = \left.\frac{\partial M}{\partial B}\right|_{B \to 0}$.

Ans Let us define the external field as ~~$\vec{H} = \mu_0 \vec{B}$~~ $\vec{H} = \frac{\vec{B}}{\mu_0}$

$\therefore$ $\boxed{\mu_0 H = B}$.

Model: We study a system of N identical, localized, practically static, mutually non interacting and freely orientable dipoles each with magnetic moment μ_i. In the presence of an external magnetic field $\vec{H}$, the dipoles will experience a torque tending to align them in the direction of field — but will however be opposed by thermal agitation in the system, which pushes for randomization at any finite temperature.

$\therefore$ Obviously, the only energy we need to consider here is the energy of the dipoles that arises from the presence of $\vec{H}$.

The energy is determined by the orientations of the dipoles wrt the direction of the field —

$$E = \sum_{i=1}^{N} E_i = -\sum_{i=1}^{N} \mu_0 \vec{\mu}_i \cdot \vec{H} = -\mu\mu_0 H \sum_{i=1}^{N} \cos\theta_i$$

∴ we can write ~~sigle~~ single particle partition function as

$$Z_1 = \sum_{\theta} e^{+\beta\mu\mu_0 H \cos\theta}$$

$$\equiv \sum_{\theta} \exp(h\cos\theta)$$ Ans

The partition function of system is then.

$$Z_N(\beta) = [Z_1(\beta)]^N$$ [As they are distinguishable, we don't ÷ by N!]

$h = \beta\mu\mu_0 H$ denotes the strength of magnetic energy $\mu\mu_0 H$ compared with thermal energy $K_B T$.

The mean magnetic moment $\vec{M}$ of the system will obviously be in direction of field $\vec{H}$.

$$\therefore \quad M_z \equiv M = N\mu \langle \cos\theta \rangle.$$

$$= N\mu \frac{\sum_{\theta} \cos\theta \exp(h\cos\theta)}{\sum_{\theta} \exp(h\cos\theta).}$$

Now,

$$\ln Z_1 = \ln\left(\sum_{\theta} \exp(\beta\mu\mu_0 H \cos\theta)\right)$$

$$\frac{\partial}{\partial H} \ln Z_1 = \frac{1}{\sum_{\theta} \exp(h\cos\theta)} \times \sum_{\theta} \mu\mu_0 \beta \cos\theta \exp(h\cos\theta).$$

$$\therefore \quad \frac{1}{\mu\mu_0\beta} \frac{\partial \ln[Z_1]}{\partial H} = \sum_{\theta} \cos\theta \exp(h\cos\theta) \Big/ \sum_{\theta} \exp(h\cos\theta).$$

Subst.

$\therefore$ Q. $M = \frac{N}{\beta\mu_0} \frac{\partial}{\partial H} \ln(Z_1(\beta))$.

$\therefore$ To determine degree of Magnetization in system, we have to find $Z_1(\beta)$?

$$Z_1(\beta) = \sum_{\theta} \exp(h\cos\theta) \sim \int \exp(h\cos\theta)\, d\Omega.$$

$$= 2\pi \times \int_0^{\pi} e^{(h\cos\theta)} \sin\theta\, d\theta$$

$$= 4\pi \frac{\sinh(h)}{h}.$$

$\therefore$

$$M = \frac{N}{\beta\mu_0} \frac{\partial}{\partial H} \ln\left(4\pi \frac{\sinh(h)}{h}\right)$$

$h = \beta\mu\mu_0 H$

$\frac{dh}{\beta\mu\mu_0} = dH$

$$= \frac{N}{\beta\mu\mu_0} \beta\mu\mu_0 \frac{\partial}{\partial h}\left[\ln(\sinh(h)) - \ln h\right]$$

$$= N\mu \underbrace{\left[\coth(h) - \frac{1}{h}\right]}_{L(x) = \coth x - \frac{1}{x}}$$ Langevin Function.

So, if we have system of N dipoles in volume V, then

$$M_z = N\mu L(h) = NM L(\beta\mu B).$$

For magnetic fields very strong (or temp. low), $h >> 1$

$L(h) \simeq 1$ $\therefore M = N\mu$ (& $\chi = 0$).

For temp. high (or weak B), $h << 1$, $L(x) \simeq \frac{x}{3} - \frac{x^3}{45} + \cdots$

upto first order given,

$$\boxed{M \simeq \frac{N\mu^2 B}{3K_B T}}$$ Ans.

$\therefore$ The low-field isothermal susceptibility is. (per unit-volume).

$$\frac{\chi}{V} = \frac{1}{V} \lim_{B\to 0} \left(\frac{\partial M}{\partial B}\right)_T = \frac{1}{V} \frac{N\mu^2}{3K_B T} = \frac{C'}{T}$$

Ans.

C' = curie constant

And this being the curie Law of Paramagnetism.

Q8) Consider a system of non-interacting spin-1/2 magnetic moments in a weak external magnetic field B. Show that to the leading order, magnetic susceptibility χ at high temp. is given by

Curie's Law: $\chi = \frac{C}{T}$.

Also compute the 2nd order correction in $1/T$ to susceptibility.

Ans. A spin-1/2 system will have $2 \times \frac{1}{2} + 1 = 2$ spin states, we denote them by discrete levels.

$s = 1$ for $\uparrow$, $s = 0$ for $\downarrow$.

In a background magnetic field $\vec{B}$, the kinetic energy picks up an extra term

$$E_{spin} = \mu_B B s \qquad \mu_B = |e|\hbar/2m. \text{ Bohr Magneton}$$

In Fermi system recall, the total no. of particles are given by

$$\frac{N}{V} = \int_0^\infty d\epsilon\ \bar{n}_{FD}(\epsilon, T)\, g(\epsilon) \rightarrow \frac{N}{V} = \frac{g_s}{\lambda^3} f_{3/2}(z).$$

Now, in presence of $\vec{B}$, energies of e- will split.

$$\frac{N_\uparrow}{V} = \frac{1}{\lambda^3} f_{3/2}\left(z e^{-\beta \mu_B B}\right)$$

$$\frac{N_\downarrow}{V} = \frac{1}{\lambda^3} f_{3/2}\left(z e^{+\beta \mu_B B}\right).$$

Our interest is to compute the magnetization, which is a measure of how the energy of system responds to magnetic field.

clearly $M = -\mu_B \underbrace{(N_\uparrow - N_\downarrow)}_{\text{Total net (\# spin up)}}$

$$= -\frac{\mu_B . V}{\lambda^3}\left[f_{3/2}\left(z e^{-\beta \mu_B B}\right) - f_{3/2}\left(z e^{\beta \mu_B B}\right) \right]$$

Now,
At high temp. and suitable low magnetic fields,

$f_{3/2}(z) \approx z$ as $z \rightarrow 0$, so that

$$M \approx \frac{2 \mu_B V z}{\lambda^3} \sinh(\beta \mu_B B)$$

Further

$$N = N_\uparrow + N_\downarrow \approx \frac{2V}{\lambda^3} \cosh(\beta \mu_B B)$$

Divide

$$M \approx \mu_B N \tanh(\beta \mu_B B)$$

The magnetic susceptibility is a measure of how easy it is to magnetise a substance. It

$$\chi = \frac{\partial M}{\partial B}$$

Now, when $T \uparrow$, B-low, $\beta \mu_B B \ll 1$

$$\tanh(\beta \mu_B B) \approx \mu_B \beta B - \frac{(\mu_B \beta B)^3}{3} + \mathcal{O}(B^5)]$$

$$\therefore \chi = \mu_B N \left[\mu_B \beta - \frac{\mu_B^3 \beta^3}{3} B^2 + \mathcal{O}(B^4) \right]$$

$$\chi = \frac{N \mu_B^2}{k_B T} - \frac{N \mu_B^4}{(k_B T)^2} B^2$$

in weak field — 2nd order correction

Q4) Consider a 3-D free electron gas at $T=0$. In the absence of magnetic field, both spin ↑ and spin ↓ states are occupied upto E_F. When B-field is turned ON, degen. is lifted.

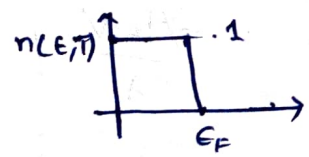
(a) Explain physically why only electrons near Fermi surface contribute to magnetisation.

(b) show that imbalance in spin populations is prop. to the density of states in Fermi level, $g(E_F)$, and to field strength B.

(c) show $M \propto g(E_F) \mu_B^2 B$.

(a) When $B=0$, $T=0$

$$N_\uparrow = N_\downarrow = \frac{1}{2} \int_0^{E_F} g(E)\, dE$$



where, $N = N_\uparrow + N_\downarrow$ ∴ we can write $g_\uparrow(E_F) = g_\downarrow(E_F) = \frac{1}{2} g(E)$.

∴ When $B=0$, both ↑ and ↓ spin e^- are degenerate.

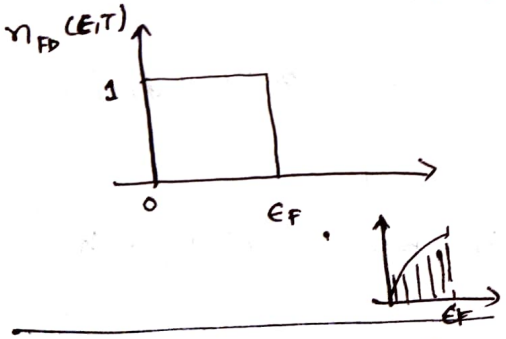
But, as ~~Before~~ B-field is turned on ($B \neq 0$)

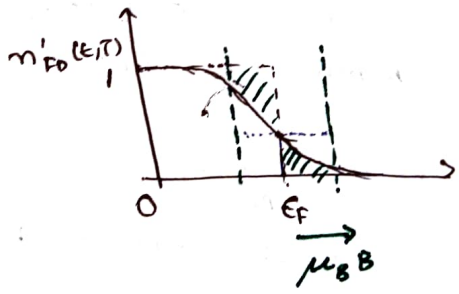
The ~~e~~ spins aligned along the $\vec{B}$ (i.e $|\uparrow\rangle$) have their energy lowered by $\mu_B B$, and those opposite (i.e $|\downarrow\rangle$) ~~lose~~ gain energy by $\mu_B B$.

However, deep inside the Fermi sea, the Pauli-Exclusion principle prevents the rearrangement of spins (in K-space), as all states are filled.

But Near surface, ~~states~~ electrons (or states) which are in the bound ($\pm \mu_B B$) around Fermi level, can make ~~transists~~ transitions to unoccupied states and contribute to magnetisation:

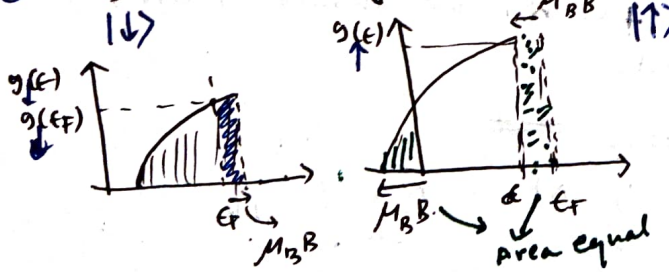
$T=0; B=0$ $\qquad$ $T=0; B \neq 0$





For 3D e^- $g(\epsilon) \sim \sqrt{\epsilon}$.

⑥ Observe Density of states





Upto 1st order, we can roughly say the imbalance in population by

$$\Delta N \sim 1 \times (+\mu_B B)\, g_{\uparrow}(\epsilon_F) + [+(\mu_B B) \times g_{\downarrow}(\epsilon_F)]$$

$$= +\mu_B B \times \tfrac{1}{2} g(\epsilon_F)$$

$$\boxed{\Delta N \propto +\mu_B B\, g(\epsilon_F)} \quad \text{or} \quad \boxed{+ B\, g(\epsilon_F)}$$ □

© Magnetisation

$$M = -\mu_B (\Delta N)$$

$$\propto -\mu_B \cdot (\mu_B B)\, g(E_F)$$

$$\propto -g(E_F)\, \mu_B^2 B \quad \square$$

Notice, it has opp. sign, $\Rightarrow$ they are repelled by magnetic fields. (unlike Pauli's paramagnetism)

Q 3) Consider a one dimensional lattice with N sites, and lattice constant - a.

$$\epsilon(k) = -2t \cos(ka), \quad k \in \left[-\frac{\pi}{a}, \frac{\pi}{a}\right)$$

(a) Find density of states $g(\epsilon)$ of system.

(b) If total No. of spinless electrons is $N_E = N/2$.

Find $\epsilon_F = ?$ $\quad g_s = 2 \times 0 + 1 = 1$ (∵ spinless) degeneracy).

Ans (a) From similar questions, recall, periodic boundary conditions ($u_{N+1} = u_1$) enforces

$$e^{ikNa} = e^{i2\pi n} \qquad n = \pm 1, \pm 2, \ldots$$

$$\rightarrow k = \frac{2\pi}{Na} n .$$

Now note, for each energy (E), $\exists$ two unique k.

s.t. $\quad E(k_1) = E(k_2), \; k_1 \neq k_2$.

∴ If we account for only +ve k, we should multiply by 2 to get total No. of states.

∴ Total No. of states, ~~having energy~~ .

$$\mathcal{N} = \sum_n \Delta n = \frac{Na}{2\pi} \sum_k \Delta k = \frac{Na}{2\pi} \int_{-\pi/a}^{\pi/a} dk$$

∴ On comparing

$$g(\epsilon) = 2 \cdot \frac{Na}{2\pi} \left| \frac{dk}{d\epsilon} \right|$$

$$\frac{d\epsilon}{dk} = +2ta\sin(ka) \rightarrow \frac{dk}{d\epsilon} = \frac{1}{a\sqrt{4t^2 - \epsilon^2}}$$

$$= 2 \times \frac{Na}{2\pi} \int_0^{2t} d\epsilon \cdot \left| \frac{dk}{d\epsilon} \right| \equiv \int g(\epsilon)\, d\epsilon .$$

$$\therefore g(\epsilon) = 2 \cdot \frac{N}{2\pi} \cdot \frac{1}{\sqrt{4t^2 - \epsilon^2}}$$

$$\boxed{g(\epsilon) = \frac{N}{\pi} \frac{1}{\sqrt{4t^2 - \epsilon^2}}} \quad \text{Ans.}$$

subst. $\sin ka = \sqrt{1 - \cos^2(ka)} = \sqrt{1 - \frac{\epsilon^2}{4t^2}}$.

check.
$$\int_{-2t}^{2t} g(\epsilon)\, d\epsilon = N$$
↑ Total No. of states.

(b) Now, we can write, the No. of states $\leq E (\leq +2t)$

as,
$$N(E) = \frac{N}{\pi} \int_{-2t}^{E} \frac{d\epsilon'}{\sqrt{4t^2 - \epsilon^2}}$$

$$= \frac{N}{\pi} \left(\sin^{-1}\left(\frac{\epsilon}{2t}\right) \right|_{-2t}^{E}$$

$$= \frac{N}{\pi} \left[\sin^{-1}\left(\frac{E}{2t}\right) + \frac{\pi}{2} \right]$$

$$N(E) = \frac{N}{\pi} \sin^{-1}\left(\frac{E}{2t}\right) + \frac{N}{2}.$$

Given, $N(E_F) = N/2$.

$$N/2 = \frac{N}{\pi}\left(\sin^{-1}\left(E_F/2t\right)\right) + N/2$$

$$\Rightarrow \sin^{-1}\left(E_F/2t\right) = 0$$

as domain of $\sin^{-1}$ is $[-1, 1]$.

$\Rightarrow E_F = 0$ but since $|\epsilon| \leq 2t \;\forall\; k$

$\therefore \boxed{E_F = 0}$ only possible!

Q5) **Artificial spin orbit coupling:**

$$\hat{H}_{1D} = \frac{1}{2m}(\hat{p}_x - \alpha\hat{\sigma}_z)^2 + \Omega\hat{\sigma}_x .$$

Ω = Rabi coupling b/w two internal spin states.

σ_z = z-component of the usual Pauli spin Matrices.

Find out the eigenvalue of above Hamiltonian and plot the corresponding dispersion relations.

Ans since it is 1D, H can be rewritten in pure momentum basis as

$$[H]_p = \frac{1}{2m}(p\,\mathbb{1} - \alpha\hat{\sigma}_z)^2 + \Omega\hat{\sigma}_x .$$

Note, p, σ_z commute with each other.

$$\therefore [H_p] = \frac{1}{2m}[p^2\mathbb{1} - 2\alpha p\hat{\sigma}_z + \alpha^2\hat{\sigma}_z^2) + \Omega\hat{\sigma}_x .$$

Subst. $\mathbb{1} = \begin{bmatrix}1 & 0\\ 0 & 1\end{bmatrix}$ $\hat{\sigma}_z = \begin{bmatrix}1 & 0\\ 0 & -1\end{bmatrix}$, $\sigma_x = \begin{bmatrix}0 & 1\\ 1 & 0\end{bmatrix}$

$$[\hat{H}]_{1D} = \begin{bmatrix}(p-\alpha)^2/2m & \Omega\\ \Omega & (p+\alpha)^2/2m\end{bmatrix}$$

Let it's eigen value be λ. We solve the characteristic equation, to calculate it's eigen values.

$$\left(\lambda - \frac{(p-\alpha)^2}{2m}\right)\left(\lambda - \frac{(p+\alpha)^2}{2m}\right) = \Omega^2$$

$$\lambda^2 - \frac{\lambda}{2m}\left[2(p^2+\alpha^2)\right] + \frac{1}{4m^2}(p^2-\alpha^2)^2 = \Omega^2 .$$

$$\lambda = \frac{1}{2}\left[\left(\frac{p^2+\alpha^2}{m}\right) \pm \sqrt{\frac{(p^2+\alpha^2)^2}{m^2} - \left[\frac{(p^2-\alpha^2)^2}{m^2} - \Omega^2\right]}\right]$$

$$= \frac{1}{2m}\left[(p^2+\alpha^2) \pm \sqrt{4(2\alpha^2)(2p^2) + m^2\Omega^2}\right]$$

$$\therefore \boxed{\lambda_\pm(p) = \frac{1}{2m}\left[(p^2+\alpha^2) \pm \sqrt{4\alpha^2p^2 + m^2\Omega^2}\right]}$$

Since these are energy eigenvalues, we replace $\lambda \to E$ and $p \to \hbar k$ to get the dispersion relations.

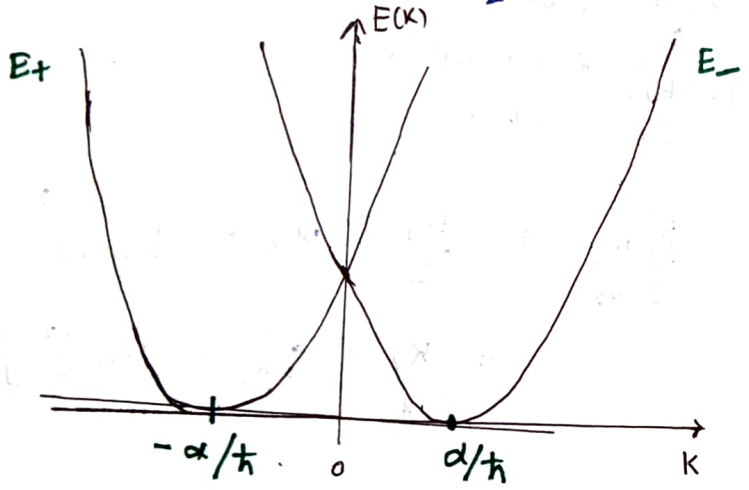
$$\left[E_\pm(k) = \frac{\hbar^2 k^2}{2m} + \frac{\alpha^2}{2m} \pm \frac{1}{2m}\sqrt{4\hbar^2 k^2 \alpha^2 + m^2\Omega^2} \right]$$

Case 1 : $\Omega = 0$

$$E_\pm(k) = \frac{\hbar^2 k^2}{2m} + \frac{\alpha^2}{2m} \pm \frac{1}{2m} \times 2\hbar k \alpha .$$

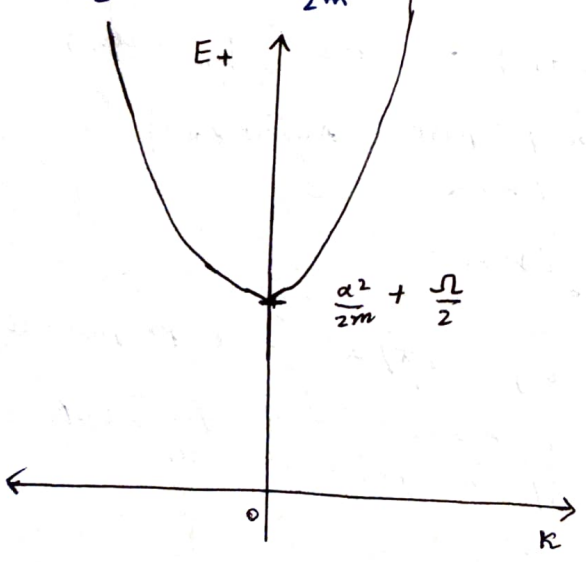
$$= \frac{1}{2m}\left[\hbar k \pm \alpha\right]^2 .$$

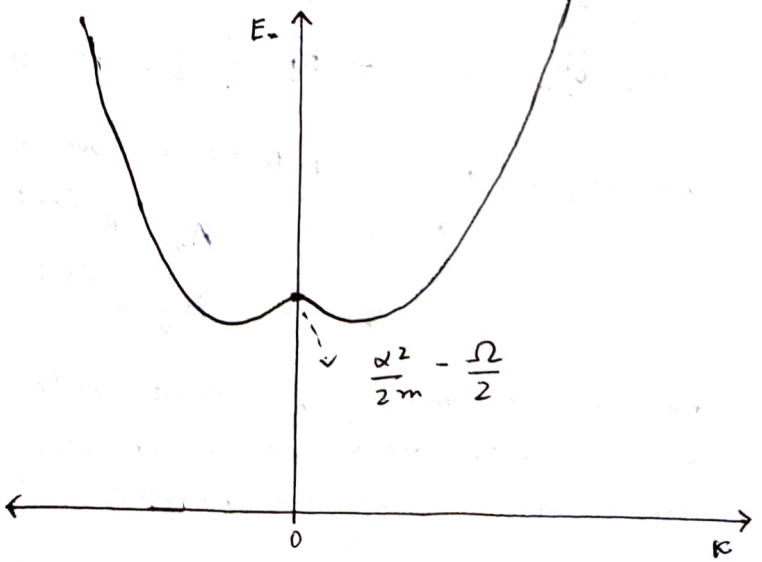
$$E_\pm(k) = \frac{\hbar^2}{2m}\left(k \pm \frac{\alpha}{\hbar}\right)^2 .$$



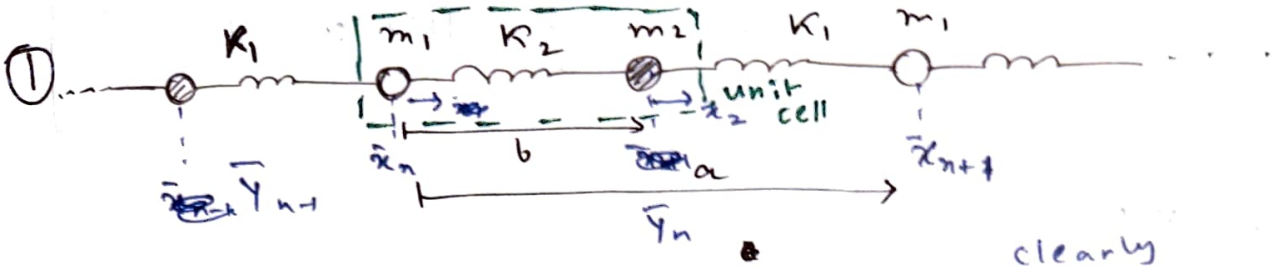
Case 2 : $\Omega \neq 0$ $(\Omega > 0)$ WLOG.

$$E_\pm(k) = \frac{\hbar^2}{2m}\left[k^2 + \frac{\alpha^2}{\hbar^2}\right] \pm \frac{2\hbar\alpha}{2m}\sqrt{k^2 + \left(\frac{m\Omega}{2\hbar\alpha}\right)^2}$$





this vanishes (0) as well, when $T \to 0$.



clearly $2b = a$

(a) Hamiltonian of system?

Let

$\bar{x}_n$, ~~$\bar{x}_{n+2}$, $\bar{x}_{n+4}$~~ .... → be eqlbm positions of m_1 masses

~~$\bar{x}_{n-1}$, $\bar{x}_{n+1}$, $\bar{x}_{n+3}$~~ ; $\bar{y}_n$ → be eqlbm positions of m_2 masses.

Let us denote instaneous position of each masses

as $x_n(t) = \bar{x}_n + u_n(t) \equiv \delta x_n$

$y_n(t) = \bar{y}_n + q_n(t)$. ↳ fluctuation

↳ $\equiv \delta y_n$.

Total Hamiltonian is

$$H = \sum_n \left[\frac{p_{1n}^2}{2m_1} + \frac{p_{2n}^2}{2m_2} + \frac{K_1}{2}(u_n - q_{n-1})^2 + \frac{K_2}{2}(q_n - u_n)^2 \right]$$

(A)

(b) Find $\omega(K) = ?$

Writing eq^{n}s of motion for system.

$$m_1 \ddot{u}_n = -K_1(u_n - q_{n-1}) - K_2(u_n - q_n)$$

$$m_2 \ddot{q}_n = -K_1(q_n - u_{n+1}) - K_2(q_n - u_n)$$

Analogous to 1-D case we can propose Ansätze.

$$u_n = A_x e^{i\omega t - iKna}$$

$$q_n = A_y e^{i\omega t - iKna}$$

Recall values of K that differ by $2\pi/a$ are physically equivalent. Here per unit cell, we have 2 d.o.f, but we obtain only one possible value of 'K' per unit cell.

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Plugging Ansatz. ~~denote $\lambda = e^{ika}$~~

$$-\omega^2 m_1 A_x e^{i\omega t - ikna} = k_2 A_y e^{i\omega t - ikna} + k_1 A_y e^{i\omega t - ik(n-1)a} - (k_1+k_2) A_x e^{i\omega t - ikna}.$$

$$-\omega^2 m_2 A_y e^{i\omega t - ikna} = k_1 A_x e^{i\omega t - ik(n+1)a} + k_2 A_x e^{i\omega t - ikna} - (k_1+k_2) A_y e^{i\omega t - ikna}.$$

simplifies to.

$$-\omega^2 m_1 A_x = k_2 A_y + k_1 A_y e^{ika} - (k_1+k_2) A_x$$
$$-\omega^2 m_2 A_y = k_1 A_x e^{-ika} + k_2 A_x - (k_1+k_2) A_y$$

$$\Rightarrow -\omega^2 A_x = A_x \times \left[-\frac{(k_1+k_2)}{m_1}\right] + A_y \left[\frac{k_2 + k_1 e^{ika}}{m_1}\right]$$
$$-\omega^2 A_y = A_x \left[\frac{k_1 e^{-ika} + k_2}{m_2}\right] + A_y \left[-\frac{(k_1+k_2)}{m_2}\right].$$

$$\Rightarrow \omega^2 \begin{pmatrix} A_x \\ A_y \end{pmatrix} = \begin{bmatrix} (k_1+k_2)/m_1 & -\frac{1}{m_1}(k_2 + k_1 e^{ika}) \\ -\frac{1}{m_2}(k_1 e^{-ika} + k_2) & \frac{k_1+k_2}{m_2} \end{bmatrix}$$

$\Rightarrow$ we expect to find non-trivial sol'n of $\begin{pmatrix} A_x \\ A_y \end{pmatrix}$ by finding zeroes of secular determinant.

$$0 = \begin{vmatrix} \frac{(k_1+k_2)}{m_1} - \omega^2 & -\frac{1}{m_1}(k_2 + k_1 e^{ika}) \\ -\frac{1}{m_2}(k_2 + k_1 e^{-ika}) & \frac{k_1+k_2}{m_2} - \omega^2 \end{vmatrix} = 0.$$

$$\left[\left(\frac{k_1+k_2}{m_1}\right) - \omega^2\right]\left[\left(\frac{k_1+k_2}{m_2}\right) - \omega^2\right] = \frac{1}{m_1 m_2} |k_1 e^{+ika} + k_2|^2.$$

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$$\omega^4 - (K_1+K_2)\left[\frac{1}{m_1}+\frac{1}{m_2}\right]\omega^2 + \frac{(K_1+K_2)^2}{m_1 m_2} - \frac{1}{m_1 m_2}\left|K_1 e^{ika} + K_2\right|^2 = 0$$

$$\omega_{\pm}^2 = \frac{1}{2}\left[(K_1+K_2)\left[\frac{1}{m_1}+\frac{1}{m_2}\right] \pm \left((K_1+K_2)^2\left(\frac{1}{m_1}+\frac{1}{m_2}\right)^2 - \frac{4}{m_1 m_2}\left[(K_1+K_2)^2 - \left|K_1 e^{ika} + K_2\right|^2\right)\right)^{1/2}\right]$$

Now

$$(K_1+K_2)^2 - K_1^2 + K_2^2 - 2K_1K_2\cos(ka)$$

$$= 2K_1K_2\left[1-\cos(ka)\right]$$

$$= 4K_1K_2\sin^2\left(\frac{ka}{2}\right).$$

∴ Clearly the dispersion relations are (ω > 0)

$$\omega_{\pm}(K) = \left\{\frac{1}{2}\left[(K_1+K_2)\left[\frac{1}{m_1}+\frac{1}{m_2}\right] \pm \left((K_1+K_2)^2\left[\frac{1}{m_1}+\frac{1}{m_2}\right]^2 - 16\frac{K_1K_2}{m_1m_2}\sin^2\left(\frac{ka}{2}\right)\right)^{1/2}\right]\right\}^{1/2}$$

(c) In limiting case

$$m = m_1 = m_2, \quad K_1 \to K_2 \to K$$

$$\omega_{\pm}(K) = \left\{\frac{1}{2}\left[2K\times\frac{2}{m} \pm \left(4K^2\times\frac{4}{m^2} - 16\frac{K^2}{m^2}\sin^2\left(\frac{ka}{2}\right)\right)^{1/2}\right]\right\}^{1/2}$$

$$= \left\{\frac{1}{2}\left[\frac{4K}{m} \pm \frac{4K}{m}\cos\left(\frac{ka}{2}\right)\right]\right\}^{1/2}$$

For ω_- —

$$\omega_-^2 = \frac{2K}{m}\left(1-\cos\frac{ka}{2}\right)$$

$$= \frac{4K}{m}\sin^2\left(\frac{ka}{4}\right) = \frac{4K}{m}\sin^2\left(\frac{Kb}{2}\right)$$

$[a = 2b]$

Thus recovering the 1D Dispersion relation, in monoatomic chain with spacing = $b = a/2$.

(d) We have

$$\omega_{\pm}^2(K) = \frac{1}{2}\left[(K_1+K_2)\left(\frac{1}{m_1}+\frac{1}{m_2}\right) \pm \sqrt{\frac{(K_1+K_2)^2}{1}\left(\frac{1}{m_1}+\frac{1}{m_2}\right)^2 \cdots - 16\frac{K_1K_2}{m_1m_2}\sin^2\left(\frac{ka}{2}\right)}\right]$$

observe as $K \to 0$

$$\omega_-^2(K) \underset{K\to 0}{=} 0 \longrightarrow \text{GAPLESS}$$

↳ long wavelength, low energy mode.

This is the sound wave / Acoustic mode.

$$v_{sound} = \frac{d\omega_-}{dK}$$

For small K,

$$\omega_-^2(K) = \frac{1}{2}\left[(K_1+K_2)\left(\frac{1}{m_1}+\frac{1}{m_2}\right) - \sqrt{(K_1+K_2)^2\left[\frac{1}{m_1}+\frac{1}{m_2}\right]^2 - \frac{16 K_1K_2}{m_1m_2}\frac{K^2a^2}{4}}\right]$$

$$\approx \frac{1}{2}\left[(K_1+K_2)\left(\frac{1}{m_1}+\frac{1}{m_2}\right) - (K_1+K_2)\left(\frac{1}{m_1}+\frac{1}{m_2}\right)\left[1 - \frac{2K_1K_2}{m_1m_2}\frac{1}{(K_1+K_2)^2}\left(\frac{1}{m_1}+\frac{1}{m_2}\right)^{-2}K^2a^2\right]\right]$$

$$\approx \left[\frac{1}{4}\cdot\frac{K_1K_2}{m_1m_2}\cdot\left(\frac{1}{K_1+K_2}\right)\left(\frac{1}{m_1}+\frac{1}{m_2}\right)^{-1}K^2a^2\right],$$

$$\omega_-^2 = \frac{K_1 K_2}{(K_1+K_2)} \cdot \frac{a^2 k^2}{(m_1+m_2)}$$

$$\therefore \boxed{\omega_-(k) = \sqrt{\frac{K_1 K_2}{(K_1+K_2)} \cdot \frac{1}{(m_1+m_2)} \cdot a^2}\, k}$$

↳ linear in k

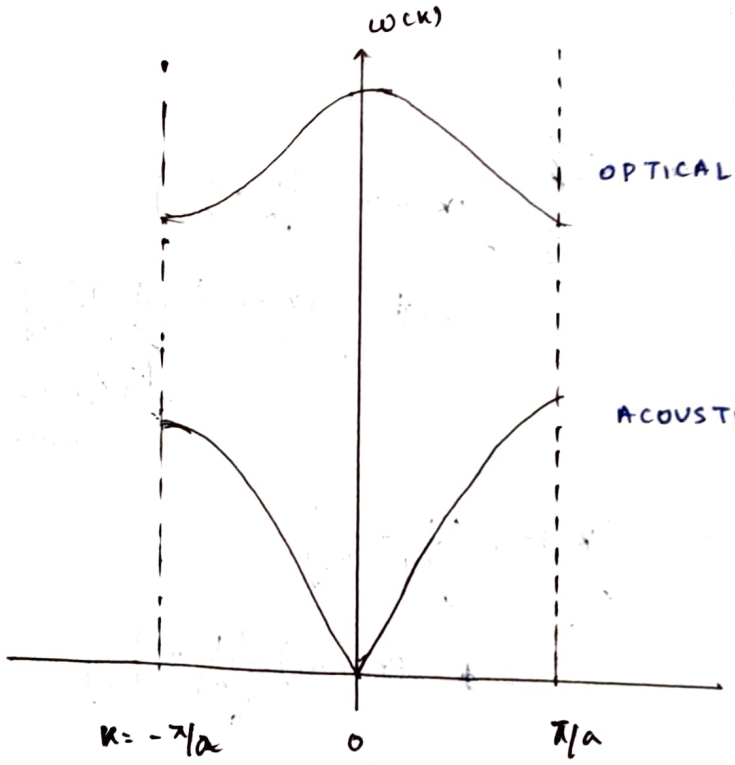
v_{sound}.

And,

for $\omega_+^2(k) \underset{k \to 0}{=} (K_1+K_2)\left(\frac{1}{m_1}+\frac{1}{m_2}\right)$ → CAPPED

this higher energy branch is called optical / capped branch.

If $m_1 = m_2 = m$.



BZ 1

Reduced Zone Scheme.