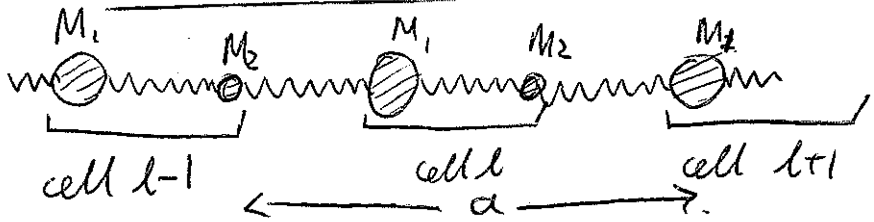
Physics 231 Homework 2 Solutions.

1/ (a)



let $\frac{a}{2}$ be spacing between the atoms

(a) M_1 is coupled to M_2 in same cell and M_2 in previous cell. Hence the equation of motion for $u_l^{(1)}$ is

(6)

$$M_1 \ddot{u}_l^{(1)} = k\left[u_l^{(2)} - u_l^{(1)} + u_{l-1}^{(2)} - u_l^{(1)}\right] \qquad (1)$$

M_2 is coupled to M_1 in same cell and M_1 in next cell, so

$$M_2 \ddot{u}_l^{(2)} = k\left[u_l^{(1)} - u_l^{(2)} + u_{l+1}^{(1)} - u_l^{(2)}\right] \qquad (2)$$

Look for a solution of the form $\begin{cases} u_l^{(1)} = \varepsilon_1 e^{i(kl-\omega t)} \\ u_l^{(2)} = \varepsilon_2 e^{i(kl-\omega t)} \end{cases}$ so

$$-M_1\omega^2 \varepsilon_1 = k\left[-2\varepsilon_1 + \varepsilon_2\left(1+e^{-ika}\right)\right]$$
$$-M_2\omega^2 \varepsilon_2 = k\left[-2\varepsilon_2 + \varepsilon_1\left(1+e^{ika}\right)\right]$$

or

$$\begin{pmatrix} M_1\omega^2 - 2k & k\left(1+e^{-ika}\right) \\ k\left(1+e^{ika}\right) & M_2\omega^2 - 2k \end{pmatrix}\begin{pmatrix} \varepsilon_1 \\ \varepsilon_2 \end{pmatrix} = 0$$

which has a solution when the determinant of the matrix vanishes, i.e.

$$\left(M_1\omega^2 - 2k\right)\left(M_2\omega^2 - 2k\right) - k^2\left(2 - 2\cos ka\right) = 0$$

$$\Rightarrow \omega^2 = \frac{k}{M_1 M_2}\left[M_1 + M_2 \pm \sqrt{(M_1+M_2)^2 - 2M_1M_2(1-\cos ka)}\right]$$

$$= \frac{k}{M_1M_2}\left[M_1 + M_2 \pm \sqrt{M_1^2 + M_2^2 + 2M_1M_2\cos ka}\right]$$

(b) When $M_1 \gg M_2$ expand in powers of $\frac{M_2}{M_1}$

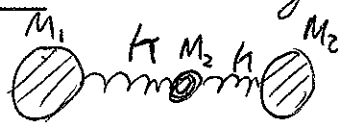
$$\omega^2 = \frac{K}{M_1 M_2} M_1 \left[1 + \frac{M_2}{M_1} \pm \sqrt{1 + \frac{2M_2}{M_1}\cos ka + \cdots} \right]$$

$$= \frac{K}{M_2}\left[1 + \frac{M_2}{M_1} \pm \left(1 + \frac{M_2}{M_1}\cos ka\right)\right] \quad \text{to 1st order in } \frac{M_2}{M_1}$$

so $\omega^2 = \frac{K}{M_1}(1 - \cos ka)$ and $\omega^2 = \frac{2K}{M_2}$ (3)

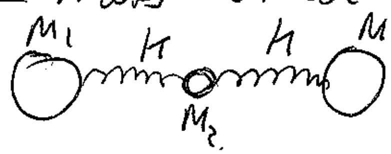
slow mode — fast mode.

For the fast mode heavy atoms don't move.



Small mass bounces backwards and forwards between the 2 heavy masses. No dispersion because each small mass vibrates independently of the others. The effective spring constant is $2K$ because there are 2 springs connected to M_2.

For the slow mode. The light atoms just follow along with the heavy atoms in such a way that the forces on the 2 springs connected to a light ~~wa~~ mass cancel (since they have the same extension)



Hence 2 neighboring heavy masses are connected effectively by 2 springs in series which have an effective spring constant $K/2$ (why?)

Hence using the result, AM (22-59) for a monatomic chain we have

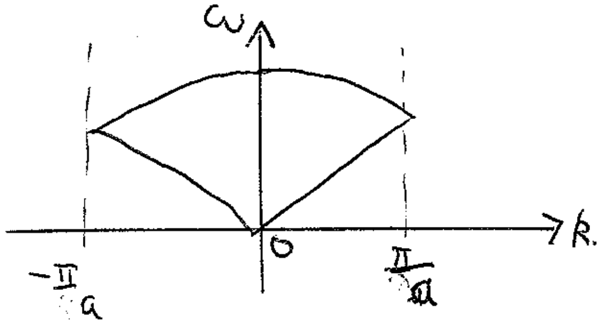
$$\omega^2 = 2\left(\frac{K}{2}\right)\frac{1}{M_1}(1 - \cos ka) = \frac{K}{M_1}(1 - \cos ka)$$

in agreement with (3).

(c) When $M_1 = M_2 = M$

$$\omega^2 = \frac{k}{MM}\left[M + M \pm \left(2M^2 + 2M^2\cos ka\right)^{1/2}\right]$$

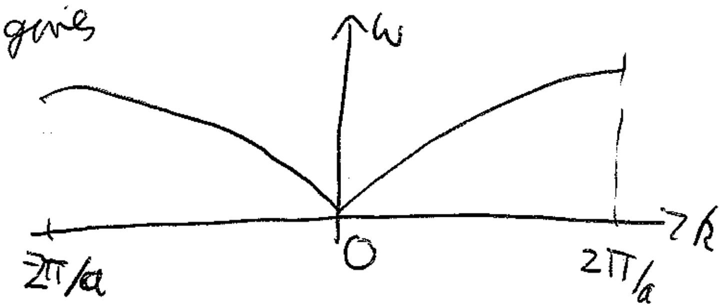
$$= \frac{k}{M}\left[2 \pm \sqrt{2+2\cos ka}\right] = \frac{2k}{M}\left[1 \pm \cos\frac{ka}{2}\right]$$



note, ~~the~~ taking the limit $M_2 \to M$, the lattice spacing is a and the BZ is $-\frac{\pi}{a} < k < \pi/a$

However for $M_2 = M_1$ the lattice spacing is really $a/2$ so we should then work in the extended zone $-\frac{2\pi}{a} < k < 2\pi/a$.

This gives



with $\omega^2 = \frac{2k}{M}\left[1 - \cos k\frac{a}{2}\right]$

in agreement with the result for a monatomic chain with lattice spacing $\frac{a}{2}$.

2/ Assume ~~also~~ neighboring atoms are connected by springs with equilibrium spacing d.

i.e. $\phi(\vec{r_i} - \vec{r_j}) = \frac{1}{2} K \left(|\vec{r_i} - \vec{r_j}| - d \right)^2$

let $\vec{r_i} = \vec{R_i} + \vec{u_i}$
$\vec{r_j} = \vec{R_j} + \vec{u_j}$ where $|\vec{R_i} - \vec{R_j}| = d$

From AM (22.11)

$$D_{\mu\nu}(\vec{R_i} - \vec{R_j}) = - \frac{\partial^2 \phi}{\partial R_\mu \partial R_\nu} \qquad (1)$$

4

Now $\phi(\vec{r}) = \frac{1}{2} K \left(|\vec{r}| - d \right)^2$ so $\frac{\partial \phi}{\partial r_\mu} = K \left(|\vec{r}| - d \right) \frac{r_\mu}{r}$

and $\frac{\partial^2 \phi}{\partial R_\mu R_\nu} = \frac{\partial^2 \phi}{\partial r_\mu \partial r_\nu} \Big|_{\vec{r} = \vec{R}} = K \frac{R_\mu R_\nu}{R^2}$ (since $|\vec{R}| - d = 0$)

$$= K \hat{R}_\mu \hat{R}_\nu \qquad (2)$$

From (1), (2) and AM. (22.59) we have.

$$M\omega^2 \epsilon^\mu = 2K \sum_R \sin^2\left(\frac{\vec{k} \cdot \vec{R}}{2}\right) \hat{R}_\mu \hat{R}_\nu \, \epsilon^\nu$$

where the sum is over the neighbors of a given lattice point.
Hence, diagonalizing the 3×3 matrix

$$\omega = \sqrt{\frac{\lambda}{M}}$$ where λ is an eigenvalue of

$$D_{\mu\nu}(\vec{k}) = 2K \sum_{\vec{R}} \sin^2\left(\frac{\vec{k} \cdot \vec{R}}{2}\right) \hat{R}_\mu \hat{R}_\nu$$

3. fcc lattice, the 12 neighbors are
$\frac{a}{2}(0, \pm 1, \pm 1)$, $\frac{a}{2}(\pm 1, 0, \pm 1)$, $\frac{a}{2}(\pm 1, \pm 1, 0)$

Hence $\hat{R}_\mu \hat{R}_\nu = \frac{1}{2}\begin{pmatrix} 1 & 1 & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix}$ ~~for $\vec{R} = \frac{a}{2}(0,1,1)$, $\frac{a}{2}(0,-1,-1)$~~ for $R = \frac{a}{2}(1,1,0)$ and $\frac{a}{2}(-1,-1,0)$

$= \frac{1}{2}\begin{pmatrix} 1 & -1 & 0 \\ -1 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix}$ ~~for $\vec{R} = \frac{a}{2}(0,1,-1)$ and~~ for $R = \frac{a}{2}(1,-1,0)$ and $\frac{a}{2}(-1,1,0)$

Similarly for the other neighbors.

(a) $\vec{k} = (k, 0, 0)$ (100) direction.

$$\sin^2\left(\tfrac{1}{2}\vec{k}\cdot\vec{R}\right) = \begin{cases} 0 & \text{for } \vec{R} = \frac{a}{2}(0, \pm 1, \pm 1) \\ \sin^2 \frac{ka}{4} & \text{otherwise} \end{cases}$$

Hence $D(\vec{k}) = 2K\sin^2\left(\frac{ka}{4}\right) \frac{1}{2}\begin{bmatrix} 8 & 0 & 0 \\ 0 & 4 & 0 \\ 0 & 0 & 4 \end{bmatrix}$ which is diagonal.

For $\mu = \hat{x}$ (i.e. longitudinal) $\lambda_\mu = 8K\sin^2\left(\frac{ka}{4}\right)$

for $\mu = \hat{y}$ and $\hat{z}$ (i.e. transverse) $\lambda_\mu = 4K\sin^2\left(\frac{ka}{4}\right)$

Hence $\underline{\omega_L = 2\sqrt{\frac{2K}{M}}\sin\left(\frac{ka}{4}\right)}$

$\underline{\omega_T = 2\sqrt{\frac{K}{M}}\sin\left(\frac{ka}{4}\right)}$ ← (2 modes)

(b) $\vec{k} = (\bar{k}, \bar{k}, \bar{k})$ i.e. (111) direction

$$\sin^2\left(\tfrac{1}{2}\vec{k}\cdot\vec{R}\right) = \begin{cases} \sin^2\left(\frac{\bar{k}a}{2}\right) & \text{for } \vec{R} = \frac{a}{2}(0,1,1),\ \frac{a}{2}(0,-1,-1) \text{ etc} \\ 0 & \text{for } R = \frac{a}{2}(0,1,-1),\ \frac{a}{2}(0,-1,1) \text{ etc} \end{cases}$$

Hence $D(\vec{k}) = 2K \sin^2\left(\frac{\bar{k}a}{2}\right) \frac{1}{2} \; 2\begin{pmatrix} 2 & 1 & 1 \\ 1 & 2 & 1 \\ 1 & 1 & 2 \end{pmatrix}$

e-vals of $\begin{pmatrix} 2 & 1 & 1 \\ 1 & 2 & 1 \\ 1 & 1 & 2 \end{pmatrix}$ are $\cancel{4}$ $\underbrace{1, \quad 1}$

e vector $\frac{1}{\sqrt{3}}(1,1,1)$ — e-vectors transverse.

i.e. longitudinal

$$\Longrightarrow \quad \omega_L = 2\sqrt{\frac{2K}{M}} \sin\left(\frac{\bar{k}a}{2}\right) \quad \text{(longitudinal)}$$

$$\omega_T = \sqrt{\frac{2K}{M}} \sin\left(\frac{\bar{k}a}{2}\right) \quad \text{(2 degenerate transverse)}$$

(c) $\vec{k} = (\bar{k}, \bar{k}, 0)$

$$\sin^2\left(\tfrac{1}{2}\vec{k}\cdot\vec{R}\right) = \begin{cases} \sin^2 \frac{\bar{k}a}{2} & \vec{R} = \frac{a}{2}(1,1,0) \text{ and } \frac{a}{2}(-1,-1,0) \\ 0 & \vec{R} = \frac{a}{2}(1,-1,0) \text{ and } \frac{a}{2}(-1,1,0) \\ \sin^2 \frac{\bar{k}a}{4} & \text{otherwise.} \end{cases}$$

Hence

$$D(\vec{k}) = 2K\left(\frac{1}{2}\right) \begin{pmatrix} 2\sin^2\frac{\bar{k}a}{2} + 4\sin^2 \bar{k}a/4, & 2\sin^2\frac{\bar{k}a}{2}, & 0 \\ 2\sin^2\frac{\bar{k}a}{2}, & 2\sin^2\frac{\bar{k}a}{2} + 4\sin^2\frac{\bar{k}a}{2}, & 0 \\ 0 & 0 & 8\sin^2\frac{\bar{k}a}{4} \end{pmatrix}$$

Hence need to diagonalize the 2×2 matrix

$$2K\begin{bmatrix} \sin^2\frac{\bar{k}a}{2} + 2\sin^2\frac{\bar{k}a}{4}, & 2\sin^2\frac{\bar{k}a}{2} \\ 2\sin^2\frac{\bar{k}a}{2}, & \sin^2\frac{\bar{k}a}{2} + 2\sin^2\frac{\bar{k}a}{4} \end{bmatrix}$$

The evalues are
$$\begin{cases} 4K \sin^2 \frac{\bar{k}a}{2} + 4K\sin^2\frac{\bar{k}a}{4}, & \text{e-vector } \frac{1}{\sqrt{2}}(1,1) \text{ i.e. longitudinal} \\ 4K \sin^2 \frac{\bar{k}a}{4}, & \text{transverse } (\perp \text{ to } z \text{ axis}) \end{cases}$$

Hence the frequencies are

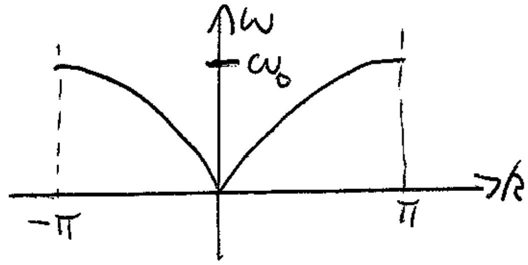
$$\omega_L = 2\sqrt{\frac{K}{M}}\left[\sin^2\frac{\bar{k}a}{2} + \sin^2\frac{\bar{k}a}{4}\right]^{1/2}$$ longitudinal

$$\omega_{T_1} = 2\sqrt{\frac{2K}{M}}\ \sin\frac{\bar{k}a}{4}$$ transverse, polarized along z-axis.

$$\omega_{T_2} = 2\sqrt{\frac{K}{M}}\ \sin\frac{\bar{k}a}{4}$$ transverse, polarized perpendicular to z-axis

9

4. $\omega = \omega_0 \sin(k/2)$ $\quad a=1$



(a) density of points / atom in k-space is $\frac{1}{2\pi}$

Hence $\rho(\omega)\,d\omega = \frac{1}{2\pi}\,dk \;(\times 2)$

Hence $\rho(\omega) = \frac{1}{2\pi}\frac{1}{d\omega/dk}\;(\times 2)$ because there are 2 values of k where ω has a certain value

$$= \frac{1}{\pi}\frac{1}{\frac{1}{2}\omega_0 \cos k/2}$$

$$= \frac{2}{\pi}\frac{1}{\sqrt{\omega_0^2-\omega^2}}$$ since $\cos k/2 = \sqrt{1-\sin^2 k/2}$

(for $0<\omega<\omega_0$)

$\rho(\omega) = 0$ outside this range

$$\frac{2}{\pi}\int_0^{\omega_0}\frac{d\omega}{\sqrt{\omega_0^2-\omega^2}} = \frac{2}{\pi}\left[\sin^{-1}\frac{\omega}{\omega_0}\right]_0^{\pi/2} = \frac{2}{\pi}\left(\frac{\pi}{2}-0\right) = 1 \;(\checkmark)$$

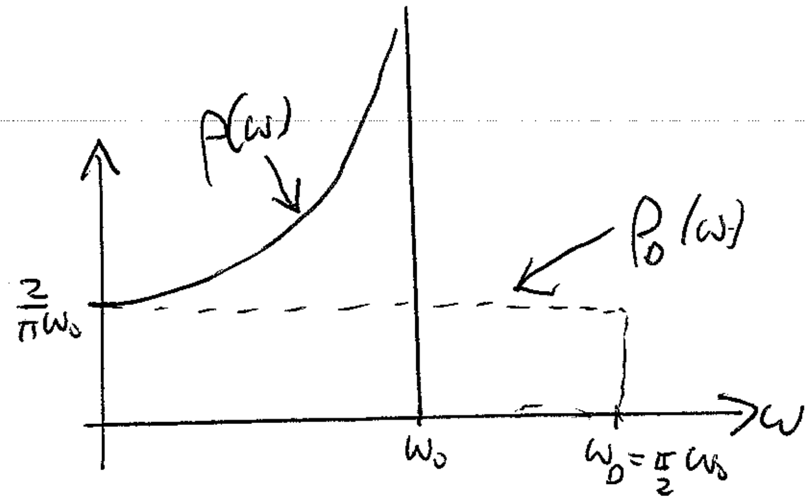
(b) the density of states diverges as $\omega \to \omega_0^-$ since the dispersion relation is flat there (see the figure above) so many states have this energy.

(c) As $\omega \to 0$ $\rho(\omega) = \frac{2}{\pi\omega_0}$

Hence $$\rho_D(\omega) = \begin{cases}\frac{2}{\pi\omega_0} & \text{for } 0<\omega<\omega_D \\ 0 & \text{otherwise}\end{cases}$$

& ω_D is determined by $1 = \int_0^{\omega_D}\rho_D(\omega)\,d\omega = \frac{2}{\pi\omega_0}\omega_D \Rightarrow \omega_D = \frac{\pi}{2}\omega_0$

(d)



(e)

$$\frac{C_D}{k_B} = \int_0^\infty \rho_D(\omega)\,\frac{e^{\beta\hbar\omega}}{(e^{\beta\hbar\omega}-1)^2}\left(\frac{\hbar\omega}{k_BT}\right)^2 d\omega$$

$$= \frac{2}{\pi\omega_0}\int_0^{\omega_D}\frac{e^{\beta\hbar\omega}}{(e^{\beta\hbar\omega}-1)^2}\left(\frac{\hbar\omega}{k_BT}\right)^2 d\omega.$$

let $x = \frac{\hbar\omega}{k_BT}$ Note $\hbar\omega_D = k_B\Theta_D$ and $\omega_D = \frac{\pi}{2}\omega_0$ so

$$\frac{C_D}{k_B} = \frac{1}{\omega_D}\int^{\Theta_D/T}\frac{x^2 e^x}{(e^x-1)^2}\;\frac{k_BT}{\hbar}\,dx.$$

$$= \frac{T}{\Theta_D}\int_0^{\Theta_D/T}\frac{x^2e^x}{(e^x-1)^2}\,dx.$$

(f) $T \to 0$, let upper limit of integrand tend to zero

$$\frac{C_D}{k_B} \doteq \frac{T}{\Theta_D}\int_0^\infty\frac{x^2e^x}{(e^x-1)^2}\,dx = \frac{T}{\Theta_D}\int_0^\infty x^2\left(e^{-x}+2e^{-2x}+3e^{-3x}+\cdots\right)dx.$$

$$= \frac{T}{\Theta_D}\,2!\left[1+\frac{2}{2^3}+\frac{3}{3^3}+\frac{4}{4^3}+\cdots\right] = \frac{T}{\Theta_D}\,2!\,\zeta(2) = \frac{\pi^2}{3}\frac{T}{\Theta_D}$$

(g) as $T \to \infty$, $\frac{\Theta_D}{T} \to 0$ so expand integrand

$$\frac{C_D}{k_B} = \frac{T}{\Theta_D} \int_0^{\frac{\Theta_D}{T}} \frac{x^2(1+\dots)}{(1+x+\dots-1)^2}\, dx = \frac{T}{\Theta_D}\int_0^{\Theta_D/T} dx = \underline{1}$$

(h) Using the exact density of states

$$\frac{C}{k_B} = \frac{2}{\pi}\int_0^{\omega_0} \frac{e^{\beta\hbar\omega}}{(e^{\beta\hbar\omega}-1)^2}\left(\frac{\hbar\omega}{k_B T}\right)^2 \frac{1}{\sqrt{\omega_0^2-\omega^2}}\, d\omega$$

let $\omega = \omega_0 \sin\theta$ so

$$\frac{C}{k_B} = \frac{2}{\pi}\left(\frac{\hbar\omega_0}{k_B T}\right)^2 \int_0^{\pi/2} \frac{e^{\sin\theta/t}}{(e^{\sin\theta/t}-1)^2} \sin^2\theta \cdot \frac{\cancel{\omega_0\cos\theta}\, d\theta}{\cancel{\omega_0\cos\theta}}$$

where $t = \frac{k_B T}{\hbar\omega_0}$

$$\text{so} \quad \frac{C}{k_B} = \frac{2}{\pi t^2}\int_0^{\pi/2} \frac{e^{\sin\theta/t}}{(e^{\sin\theta/t}-1)^2} \sin^2\theta\, d\theta$$

(i) $t \to \infty$, expand $e^{\sin\theta/t}$ so

$$\frac{C}{k_B} = \frac{2}{\pi t^2}\int_0^{\pi/2} \frac{1 \quad \sin^2\theta}{\sin^2\theta/t^2}\, d\theta = \frac{2}{\pi}\int_0^{\pi/2} 1\, d\theta$$

$$= \underline{\underline{1}} \quad \text{(the Dulong-Petit law)}$$

$t \to 0$ Only the small θ region contributes significantly and upper limit can be sent to ∞

$$\Rightarrow \frac{C}{k_B} = \frac{2}{\pi t^2}\int_0^{\infty} \frac{e^{\theta/t}}{(e^{\theta/t}-1)^2}\, \theta^2\, d\theta.$$

let $\theta/t = x$

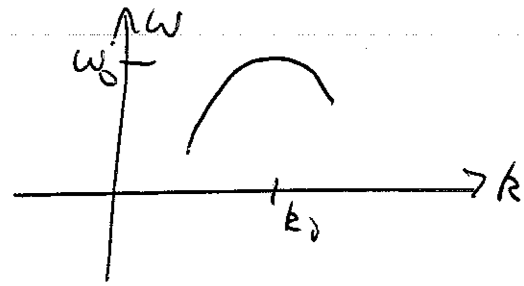
$$\Rightarrow \frac{C}{k_B} = \frac{2}{\pi \cancel{t^2}}\int_0^{\infty} \frac{e^x}{(e^x-1)^2}\, x^2\, dx\, \cancel{t^3}.$$

This is the same expression found in the Debye theory

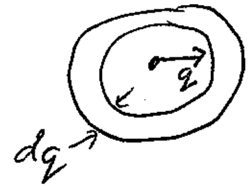
Hence Debye theory results are correct in this limit.

5. Near the maximum let

$$\omega = \omega_0 - A|\vec{k}-\vec{k_0}|^2 \quad \text{where } A>0$$



d=2 let $\vec{k}-\vec{k_0} = q$.



Number of states (per atom) in the ring between q and $q+dq$ is

$$\frac{1}{N}\frac{V}{(2\pi)^2} 2\pi q\, dq$$

$$\omega = \omega_0 - Aq^2$$
$$d\omega = -2Aq\, dq$$

Hence

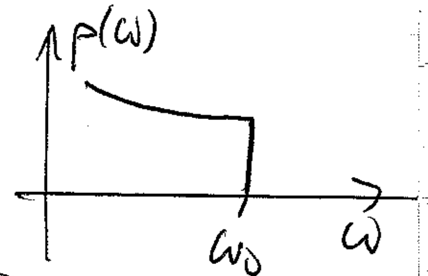
$$\rho(\omega)\, d\omega = \frac{1}{n\, 2\pi} q\, dq$$

4

$$\rho(\omega) = \frac{1}{2\pi n}\left|q\frac{dq}{d\omega}\right| = \frac{1}{2\pi n}\frac{1}{2A} \quad \text{i.e. const for } \omega<\omega_0$$

For $\omega > \omega_0$ there are no states so $\rho(\omega) = ~~\infty~~\, 0$

Hence there is a discontinuity in the density of states



d=3

number of states ~~on a~~ (per atom) in a ~~ster~~ spherical shell between q and $q+dq$ is

$$\frac{1}{N}\frac{V}{(2\pi)^3} 4\pi q^2\, dq$$

Hence $\rho(\omega)\, d\omega = \frac{1}{2\pi^2 n} q^2\, dq$

$$\rho(\omega) = \frac{1}{2\pi^2 n}\frac{q^2}{|d\omega/dq|} = \frac{1}{2\pi^2 n\, 2A} q$$

But $q \propto (\omega_0-\omega)^{1/2}$ so $\rho(\omega) \sim \begin{cases} (\omega_0-\omega)^{1/2}, & \omega<\omega_0 \\ 0 & \omega>\omega_0 \end{cases}$