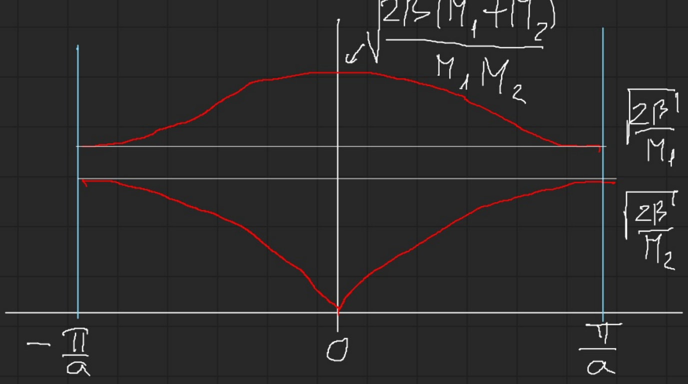
Lecture #16

Specific heat of solids

$\boxed{1D}$ Monatomic linear chain $\omega(k) = 2\sqrt{\frac{\beta}{M}}\left|\sin\frac{1}{2}ka\right|$

Diatomic —||— $\omega(k)_{\pm} = \frac{\beta}{M_1M_2}\sqrt{m^2 - 4M_1M_2\sin^2 k\frac{a}{2}}$)

$m = M_1 + M_2$



Classical physics $\frac{1}{2}k_BT$ fr

Classical physics: $\mathcal{E} = \frac{N}{2}k_BT\cdot f$ f - degree of freedom

N molecule $= \frac{N}{2L_A}L_Ak_BT\cdot f = \frac{f}{2}\cdot MRT$ $R = 8{,}31\,\frac{J}{mol\,K}$

ideal gas unit

examples:

monatomic $\varepsilon = \frac{1}{2} m (v_x^2 + v_y^2 + v_z^2) \rightarrow f = 3$ $\quad U = \frac{3}{2} MRT$

diatomic $\varepsilon = \frac{1}{2} m \underbrace{(v_x^2 + v_y^2 + v_z^2)}_{3} + \underbrace{\frac{1}{2}\Theta_1 \omega_1^2 + \frac{1}{2}\Theta_2 \omega_2^2}_{2}$

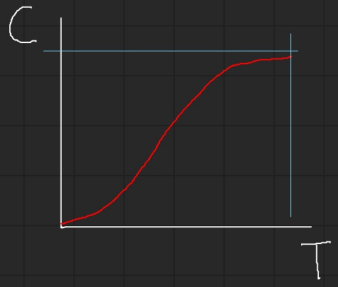
$f = 5 \quad U = \frac{5}{2} MRT$

$C_V = \left(\frac{\partial U}{\partial T}\right)_{V=\text{const}}$ heat capacity per mole

$$C = \frac{1}{M}\left(\frac{\partial U}{\partial T}\right) = \begin{cases} \frac{3}{2} R \\ \frac{5}{2} R \end{cases} = \frac{f}{2} R$$

What happens when $T \rightarrow 0$? Nothing...

Reality:



\# of phonon states

$$dn_s(\nu, \nu + d\nu) = \frac{4\pi V}{v_s^3(\nu)} \nu^2 \, d\nu \qquad v_s = \begin{cases} v_{\text{longitudinal}} \\ v_{\text{transversal}} \end{cases}$$

$$dn(\nu, \nu + d\nu) = \underbrace{4\pi V \nu^2 \left(\frac{1}{v_l^3(\nu)} + \frac{2}{v_t^3(\nu)}\right)}_{g_{\text{total}}(\nu)} d\nu$$

N atoms $\Rightarrow f = 3N \equiv$ (tot. # of states)

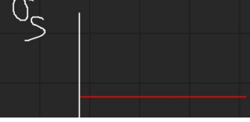
$$\Updownarrow$$

$$\int_0^\infty dn = \int_0^\infty g_{\text{tot}}(\nu)\, d\nu$$

$$4\pi V \int_0^\infty \left(\frac{1}{v_l^3(\nu)} + \frac{2}{v_t^3(\nu)}\right) \nu^2 \, d\nu = 3N$$

can't calculate!

Debye assumptions



$$\underline{\underline{g}}$$

$$v_l, v_t$$

$$4\pi V\left(\frac{1}{v_l^3}+\frac{2}{v_t^3}\right)\underbrace{\int_0^{\nu_D}\nu^2 d\nu}_{\left[\frac{\nu^3}{3}\right]_0^{\nu_D}=\frac{\nu_D^3}{3}}=3N$$

$$\frac{1}{v_l^3}+\frac{2}{v_t^3}=\frac{9N}{4\pi V\nu_D^3}$$

$$g(\nu)=\frac{9N}{\nu_D^3}\nu^2$$

\# of phonons?

$$dn=g(\nu)f_{BE}(\nu)\,d\nu$$

$$f_{BE}=\frac{\nu^2\,d\nu}{e^{h\nu/k_BT}-1}$$

$$U=\int_0^{\nu_D}\underset{h\nu}{\varepsilon(\nu,T)}\,g(\nu)f_{BE}(\nu,T)\,d\nu+\text{const.}$$

$$U=\frac{9Nh}{\nu_D^3}\int_0^{\nu_D}\frac{\nu^3}{e^{h\nu/k_BT}-1}d\nu+\text{const.}$$

$$C_V=\left(\frac{\partial U}{\partial T}\right)_{V=\text{const}}\qquad \frac{\partial}{\partial T}\int(\dots)d\nu=\int\frac{\partial}{\partial T}(\dots)d\nu$$

$$\frac{\partial}{\partial T}\frac{\nu^3}{e^{h\nu/k_BT}-1}=\frac{\nu^4e^{h\nu/k_BT}}{\left(e^{h\nu/k_BT}-1\right)^2}$$

$$\Theta_D:=\frac{h\nu_D}{k_B}\qquad C_V=9R\left(\frac{T}{\Theta_D}\right)^3\int_0^{\Theta_D/k_BT}\frac{y^4e^y}{(e^y-1)^2}dy$$

$C_V \sim T^3$ if $T \ll \Theta_D$

$C_V \sim 3R$ $\quad T \gg \Theta_D \Leftarrow$ Classical physics:

$f = 2 \cdot 3$ $\quad \big(\underbrace{\tfrac{1}{2} m v^2 + \tfrac{1}{2} D x^2}_{x,y,z}\big)$

$C_V = \frac{6}{2} R$

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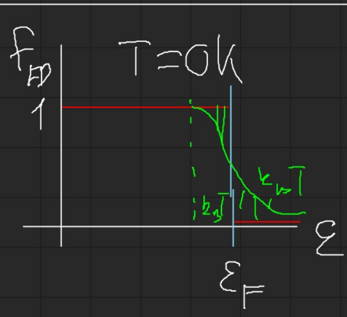
electrons?



# of electrons

$U \sim (k_B T)^2$

$C_V^{(e)} \sim T$

$$\frac{C_V^{(e)}}{C_V^{l}} \approx$$

$x^2)$

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