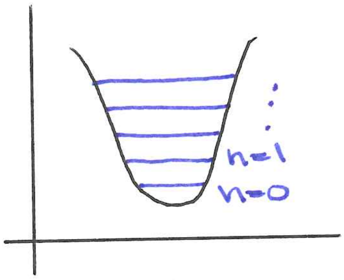
F6 FONONER

$$E_n = \left(n + \tfrac{1}{2}\right)\hbar\omega \qquad n = 0, 1, 2, \dots$$

Nollpunktsenergi: $\frac{1}{2}\hbar\omega$



$n=0$

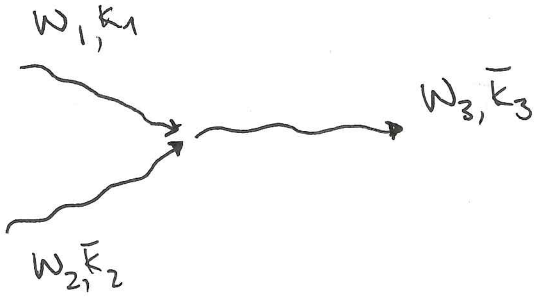
$n=n_1$

$n>n_1$

Bose-Einstein statistik

fononer vid en viss temperatur och frekvens (ω)

$$f_{BE}(\omega, T) = \frac{1}{e^{\hbar\omega/k_BT} - 1}$$



$$\begin{cases} \omega_1 + \omega_2 = \omega_3 \\ \bar{k}_1 + \bar{k}_2 = \bar{k}_3 \end{cases}$$

$|k|$ inom $\left[-\frac{\pi}{a}, \frac{\pi}{a}\right]$

om $|k_3| > \frac{\pi}{a}$ → subtrahera/addera en vektor $\frac{2\pi}{a} \cdot n$

Mätning m. { Infraröd ~~spridning~~ spektroskopi (IR) (förändring i dipolmoment)
Raman spektroskopi (förändring i polaris-abilitet)

Värmekapacitet

Fononers bidrag till värmekap., C_p

Beräkna först bidraget från <u>en</u> fonon, och summera över alla existerande

Medelenergi för en fonon:

$$\bar{\varepsilon} = \frac{\sum_n P_n \varepsilon_n}{\sum_n P_n}$$

$\varepsilon_n = (n + \frac{1}{2})\hbar\omega$

$P_n =$ Sannolikhet att fononen är på denna nivå

P_n ges av Boltzmann-statistik $\left(\exp\left(-\varepsilon_n / k_B T\right)\right)$

$$\bar{\varepsilon} = \frac{\sum_{n=0}^{\infty} (n+\frac{1}{2})\hbar\omega \exp\left(\frac{-(n+\frac{1}{2})\hbar\omega}{k_B T}\right)}{\sum_0^{\infty} \exp\left(\frac{-(n+\frac{1}{2})\hbar\omega}{k_B T}\right)}$$

sätt $\quad Z = \sum_0^{\infty} \exp\left(\frac{-(n+\frac{1}{2})\hbar\omega}{k_B T}\right)$

$$\frac{dZ}{dT} = \sum_0^{\infty} (n+\frac{1}{2})\hbar\omega / k_B T^2 \exp\left(\frac{-(n+\frac{1}{2})\hbar\omega}{k_B T}\right)$$

$$= \frac{1}{k_B T^2} \sum (n+\frac{1}{2}) \exp\left(\frac{-(n+\frac{1}{2})\hbar\omega}{k_B T}\right)$$

$$\bar{E} = k_B T^2 \cdot \frac{1}{Z}\frac{\partial Z}{\partial T} = k_B T^2 \frac{d(\ln Z)}{dT}$$

$$Z = \sum_0^\infty \exp\left(\frac{-(n+\frac{1}{2})\hbar\omega}{k_B T}\right) = \exp\left(\frac{-\hbar\omega}{2k_B T}\right)\sum_0^\infty \exp\left(\frac{-n\hbar\omega}{k_B T}\right)$$

$$\left\{\begin{array}{l} \text{sätt} \quad x = \exp\left(\frac{-\hbar\omega}{k_B T}\right) \\ x < 1 \rightarrow \sum_0^\infty x^n = \frac{1}{1-x} \end{array}\right\}$$

$$Z = \exp\left(\frac{-\hbar\omega}{2k_B T}\right)\sum \exp\left(\frac{-n\hbar\omega}{k_B T}\right) = \exp\left(\frac{-\hbar\omega}{2k_B T}\right)\frac{1}{1-\exp\left(\frac{-\hbar\omega}{k_B T}\right)}$$

$$\ln(Z) = -\frac{\hbar\omega}{k_B T} + \ln\left(\frac{1}{1-\exp\left(\frac{-\hbar\omega}{k_B T}\right)}\right)$$

$$= -\frac{\hbar\omega}{k_B T} + \ln(1) - \ln\left(1-\exp\left(\frac{-\hbar\omega}{k_B T}\right)\right) = \ln Z$$

$$\bar{E} = k_B T^2 \frac{\partial(\ln Z)}{\partial T} = k_B T^2 \frac{\partial}{\partial T}\left(\frac{-\hbar\omega}{2k_B} - \ln(1-x)\right)$$

$$= k_B T^2\left[\frac{\hbar\omega}{2k_B T^2} - \frac{\hbar\omega}{k_B T^2}\,\frac{x}{1-x}\right]$$

Div. med $x = \exp\left(\frac{-\hbar\omega}{k_B T}\right) \rightarrow \bar{E} = \frac{1}{2}\hbar\omega + \frac{\hbar\omega}{\exp\left(\frac{\hbar\omega}{k_B T}\right)-1}$

$$\bar{\varepsilon} = \underbrace{\frac{1}{2}\hbar\omega}_{\text{Nollpunktsenergin}} + \frac{\hbar\omega}{\exp\left(\frac{\hbar\omega}{k_B T}\right) - 1}$$

$$T \text{ låg} \Rightarrow \bar{\varepsilon} = \frac{1}{2}\hbar\omega$$

$$T \text{ hög} \Rightarrow \bar{\varepsilon} = \frac{1}{2}\hbar\omega + \frac{\hbar\omega}{1 + \frac{\hbar\omega}{k_B T} + \frac{1}{2}\left(\frac{\hbar\omega}{k_B T}\right)^2 + \ldots - 1}$$

$$= \frac{1}{2}\hbar\omega + \frac{\hbar\omega}{\frac{\hbar\omega}{k_B T}\left(1 + \frac{1}{2}\frac{\hbar\omega}{k_B T} + \ldots\right)}$$

$$= \frac{1}{2}\hbar\omega + k_B T\left(1 - \frac{1}{2}\frac{\hbar\omega}{k_B T} + \ldots\right)$$

$$\left\{ \sum_0^\infty x^n = \frac{1}{1-x} \right\}$$

$$\Rightarrow \bar{\varepsilon} = \frac{1}{2}\hbar\omega + k_B T\left(1 - \frac{1}{2}\frac{\hbar\omega}{k_B T} + \ldots\right)$$

$$= \frac{1}{2}\hbar\omega + k_B T - \frac{1}{2}\hbar\omega \simeq \boxed{k_B T = \varepsilon_n}$$

$$C = \frac{d\bar{\varepsilon}}{dT} = \frac{d}{dT}\left(\frac{1}{2}\hbar\omega + \frac{\hbar\omega}{\gamma - 1}\right) \qquad \left\{ \gamma = \exp\left(\frac{\hbar\omega}{k_B T}\right) \right\}$$

$$= \frac{d}{dT}\left(\frac{\hbar\omega}{\gamma - 1}\right) = -\hbar\omega\left(\frac{-\hbar\omega}{k_B T^2}\right)(\gamma - 1)^2 \gamma$$

$$c = \left(\frac{\hbar\omega}{T}\right)^2 \cdot \frac{1}{k_B} \frac{\gamma}{(\gamma-1)^2}$$

Låt $\frac{\hbar\omega}{k_B} = \theta$

$$c = \left(\frac{\theta}{T}\right)^2 k_B \frac{\exp\left(\frac{\theta}{T}\right)}{\left(\exp\left(\frac{\theta}{T}\right)-1\right)^2}$$

{ Värmekapacitet för en fonon }

Vid hög T $\left\{ \begin{array}{l} c \to k_B \\ \frac{d}{dT} \varepsilon_{Hög} = \frac{d}{dT}(k_B T) \end{array} \right.$

Värmekap för hela kristallen?

N atomer

Antar att atomerna vibrerar med samma frekvens

$$c^{\text{hel kristall}}_{\text{Hög } T} = k_B \cdot 3N$$ Einstein, ok vid höga T!

Vad är ~~distr. frekvensen~~ distributionen av vibrationsfrekvensen?

Tillståndstäthet $D(\omega)$ = # fononer som funktion av fononers frekvens!

$D(\omega)$ i 1D?

1D linjär, enatomig kedja

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

$$D(\omega)\,d\omega = 2N(k)\,dk$$

$D(\omega)\,d\omega$ = # fonontillstånd med en hög frekvens inom intervallet kring ω

$N(k)\,dk$ = # k-värden vid k inom dk

$$D(\omega) = 2N(k)\frac{dk}{d\omega} = 2N(k)\left(\frac{d\omega}{dk}\right)^{-1}$$

$$\omega = \sqrt{\frac{4c}{m}}\left|\sin\left(\frac{ka}{2}\right)\right| \rightarrow \frac{d\omega}{dk} = a\sqrt{\frac{c}{m}}\cos\left(\frac{ka}{2}\right)$$

$$\begin{cases} \omega^2 = \dfrac{4c}{m}\sin^2\left(\dfrac{ka}{2}\right) \\ \sin^2\left(\dfrac{ka}{2}\right) + \cos^2\left(\dfrac{ka}{2}\right) + 1 \end{cases} \qquad \begin{cases} \sin^2\left(\dfrac{ka}{2}\right) = \dfrac{\omega^2 m}{4c} \\ \cos\left(\dfrac{ka}{2}\right) = \sqrt{1-\sin^2\left(\dfrac{ka}{2}\right)} \end{cases}$$

$$\frac{d\omega}{dk} = a\sqrt{\frac{c}{m}}\sqrt{1-\sin^2\left(\frac{ka}{2}\right)} = a\sqrt{\frac{c}{m}}\sqrt{1-\frac{\omega^2 m}{4c}}$$

$$= \ldots = \frac{a}{2}\sqrt{\frac{4c}{m}-\omega^2}$$

$$D(\omega) = 2N(k)\underbrace{\left(\frac{d\omega}{dk}\right)^{-1}}_{\frac{a}{2}\sqrt{\frac{4c}{m}-\omega^2}}$$

$\{L = N \cdot a\}$

Antag $\begin{cases} N+1 \text{ atomer} \\ \text{Periodiska randvillkor} \end{cases}$

$$\begin{cases} u_s = u_0 \exp(i(\overbrace{ksa}^{\sigma} - \omega t)) \\ u_{s=1} = u_{s=N+1} \end{cases}$$

$$u_0 \exp(i\sigma) = u_0 \exp(i(k(N+1)a - \omega t))$$

$$\rightarrow e^{ikNa} = 1 \rightarrow kNa = 2\pi \cdot n$$

$$k = \frac{2\pi}{Na} n = \frac{2\pi}{L} n$$

$$N(k) = \frac{1}{2\pi/L} = \frac{L}{2\pi}$$

$$D(\omega) = 2N(k)\left(\frac{d\omega}{dk}\right)^{-1} = 2\,\frac{L}{2\pi}\cdot\frac{2}{a}\sqrt{\frac{1}{\frac{4c}{m}-\omega^2}}$$

$$= \frac{2N}{\pi}\,\frac{1}{\sqrt{\frac{4c}{m}-\omega^2}} = D(\omega)$$

Medelenergi för en fonon

$$\bar{E} = \frac{1}{2}\hbar w + \frac{\hbar w}{\exp\left(\frac{\hbar w}{k_B T}\right) - 1}$$

Tot energi i 1D

$$E = \int_0^\infty \left(\frac{1}{2}\hbar w + \frac{\hbar w}{\exp\left(\frac{\hbar w}{k_B T}\right) - 1} \right) D(w)\, dW$$

$$C = \frac{dE}{dT}$$