Classical Harmonic oscillator :

first, recall ~~canonical~~ the result from canonical ensemble :

$$Z(N) = \left[\frac{T}{\hbar\omega}\right]^{dN} \Rightarrow \text{specific heat } c = \frac{1}{N}\frac{dE}{dT} = d = \text{indep. of } T.$$

Grand Canonical :

$$\mathcal{Q} = \sum_N Z(N)\, e^{\beta\mu N}$$

$$= \frac{1}{1 - \frac{T}{\hbar\omega} e^{\beta\mu}} = e^{-\beta\mathcal{G}}$$

$$d\mathcal{G} = -S\,dT - N\,d\mu$$

$$\Rightarrow N = -\frac{\partial\mathcal{G}}{\partial\mu} = -\frac{\partial}{\partial\mu} T \log\left[1 - \frac{T}{\hbar\omega} e^{\beta\mu}\right]$$

$$= \frac{T}{1 - \frac{T}{\hbar\omega} e^{\beta\mu}} \times \frac{T}{\hbar\omega} e^{\beta\mu}\beta$$

$$= \frac{T/\hbar\omega\, e^{\beta\mu}}{1 - T/\hbar\omega\, e^{\beta\mu}}$$

$$= \frac{1}{\frac{\hbar\omega}{T} e^{-\beta\mu} - 1}$$

Note that N has nothing to do with the Bose-Einstein distribution in the classical limit. Here N corresponds to the # of distinct SHO's while $n = \frac{1}{e^{\beta(\varepsilon-\mu)} - 1}$ in B.E. dist. corresponds to the # of quanta of a single SHO.

A Single Quantum Harmonic Oscillator

$$\hat{H} = \omega(a^\dagger a + \tfrac{1}{2})$$

$$a = \sqrt{\frac{m\omega}{2}}\left[\hat{x} + \frac{i\hat{p}}{m\omega}\right]$$

Hilbert space ~~size~~ : countably infinite.

eigenstates : $\hat{H}\,|n\rangle = \omega n\,|n\rangle$

(recall :
$$\left.\begin{aligned} a^\dagger |n\rangle &= \sqrt{n+1}\,|n+1\rangle \\ a\,|n\rangle &= \sqrt{n}\,|n-1\rangle \end{aligned}\right\} \text{Ladder operators}$$

$$Z = \mathrm{Tr}\, e^{-\beta\hat{H}}$$ (neglecting zero point energy)

$$= \sum_{n=0}^{\infty} \langle n|\, e^{-\beta\omega a^\dagger a}\,|n\rangle$$

$$= \sum_{n=0}^{\infty} e^{-\beta\omega n} = \frac{1}{1-e^{-\beta\omega}} \qquad \text{(Eq. 29)}$$

$$\langle n\rangle = \sum_n n\, e^{-\beta\omega n} \Big/ \sum_n e^{-\beta\omega n}$$

$$= \frac{-\partial \log Z}{\partial(\beta\omega)}$$

$$= \frac{\partial \log\left[1-e^{-\beta\omega}\right]}{\partial(\beta\omega)} = \frac{e^{-\beta\omega}}{1-e^{-\beta\omega}} = \boxed{\frac{1}{e^{\beta\omega}-1}}$$

"Bose-Einstein distribution."

Grand canonical Ensemble for a $\underline{\text{single}}$ quantum SHO:

$$\mathcal{Q} = \mathrm{Tr}\ e^{-\beta[\hat{H} - \mu\hat{N}]}$$

where $\hat{H} = (a^\dagger a + \frac{1}{2})$ and $\hat{N} = a^\dagger a$ counts the # of excitations of the oscillator. $\hat{N}$ <u>does not</u> correspond to # of distinct oscillators (we are working with a <u>single</u> oscillator).

$$\Rightarrow \quad \mathcal{Q} = \sum_n \langle n| e^{-\beta[a^\dagger a\,\omega - \mu a^\dagger a]} |n\rangle$$

(again neglecting zero point energy)

$$= \sum_n e^{-\beta(\omega-\mu)n} = \frac{1}{1 - e^{-\beta(\omega-\mu)}}$$

<u>Correspondence with classical harmonic oscillator</u>

Consider a <u>single</u> classical SHO in canonical ens.:

$$Z_{cl} = \frac{T}{\hbar\omega} \quad \text{as discussed above (in } d=1).$$

while

$$\underset{\text{quantum}}{Z_{Q}} = \frac{1}{1 - e^{-\beta\hbar\omega}} \longrightarrow \frac{T}{\hbar\omega} \quad \text{when } T \gg \hbar\omega$$

Therefore, one recovers classical result when $T \gg \hbar\omega$.

One can therefore go ahead and study the quantum oscillator in the two limits: $T \gg \hbar\omega$ (classical limit) and $T \ll \hbar\omega$ ("quantum" limit):

free energy: $F = -T \log Z_Q$

for a single quantum oscillator. $= T \log[1 - e^{-\beta\omega}]$

Entropy $S = -\dfrac{dF}{dT}$

consider two limit, $T \gg \hbar\omega$, $T \ll \hbar\omega$

$T \gg \hbar\omega$ $\quad F \simeq T \log\left[\dfrac{\omega}{T}\right]$

$\Rightarrow S \simeq -\log\left[\dfrac{\omega}{T}\right] + 1$

$\Rightarrow$ specific heat $C = T\dfrac{dS}{dT} \simeq 1$

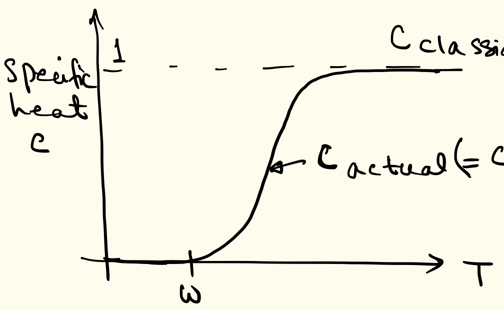
equipartition "theorem".

$T \ll \hbar\omega$ $\quad F \simeq -T e^{-\beta\omega}$

$S \simeq e^{-\beta\omega} + T e^{-\beta\omega} \dfrac{\omega}{T^2}$

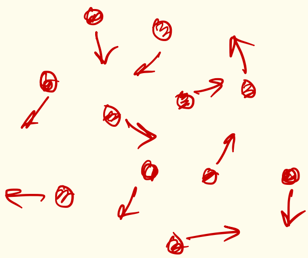
$C = T\dfrac{dS}{dT} \simeq T e^{-\omega\beta} \dfrac{\omega}{T^2} + \dfrac{\omega}{T} e^{-\beta\omega} \dfrac{\omega}{T^2} T - \dfrac{\omega}{T^2} T e^{-\beta\omega}$

$= \dfrac{\omega^2}{T^2} e^{-\beta\omega}$

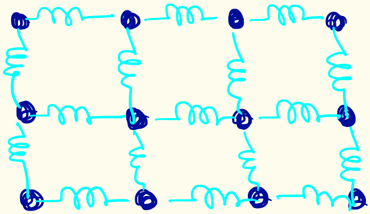


Lattice Vibrations ('Phonons')
&
Specific Heat of Solids

As briefly alluded to in the first lecture, a solid crystal breaks the continuous translation symmetry of space to discrete translation symmetry.



Liquid

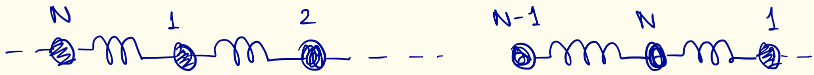


Solid crystal

There is a general result which states that whenever a continuous symmetry is spontaneously broken (we will discuss in detail later what does 'spontaneous' means here), it results in excitations whose energy-momentum relation is of the form: $\varepsilon(\vec{p}) = c\,|\vec{p}|^{\alpha}$ with α a positive integer (typically $\alpha = 1$ or $\alpha = 2$). Such an excitation is called a Goldstone mode.

Let us study a simple example which illustrates this.

Consider a system of coupled Harmonic oscillators:



We model it via the following Hamiltonian:

$$\hat{H} = \sum_{i=1}^{N} \frac{\hat{p}_i^2}{2m} + \frac{1}{2} m \omega_0^2 \sum_{i=0}^{N} (\hat{x}_i - \hat{x}_{i+1})^2$$

with $\hat{x}_{N+1} = \hat{x}_1$

The Heisenberg's equations of motion are:

$$\frac{d\hat{p}_i}{dt} = m\omega_0^2 (\hat{x}_{i+1} + \hat{x}_{i-1} - 2\hat{x}_i)$$

$$\Rightarrow m\frac{d^2\hat{x}_i}{dt^2} = m\omega_0^2 (\hat{x}_{i+1} + \hat{x}_{i-1} - 2\hat{x}_i)$$

$\left[k = \frac{2\pi m}{N},\ m = 0 - N-1\right]$

Fourier transforming:

$$\hat{x}_k = \frac{1}{\sqrt{N}} \sum_i \hat{x}_i e^{-ik \cdot r_i}$$

(r_i = mean location of $\hat{x}_i$)

$$\Rightarrow \frac{d^2\hat{x}_k}{dt^2} = \omega_0^2 \hat{x}_k (e^{-ik \cdot a} + e^{ika} - 2)$$

$$= -4\omega^2 \sin^2\left(\frac{ka}{2}\right) \hat{x}_k$$

$$\Rightarrow \boxed{\frac{d^2\hat{x}_k}{dt^2} + 4\omega^2 \sin^2\left(\frac{ka}{2}\right)\hat{x}_k = 0}$$

Thus, the system decomposes into N 'normal modes' (= decoupled harmonic oscillators) with frequencies:

$$\omega_k = 2\omega_0 \sin\left(\frac{ka}{2}\right) \qquad k = \frac{2\pi n}{N},$$
$$n = 0, 1, 2, \ldots N-1.$$

Note that $k=0$ mode just corresponds to translating the whole system rigidly (i.e. without any internal motion).

These modes are Goldstone modes! $\equiv$ sound modes / vibrational modes.

At low frequency,

$$\omega_k \sim \omega_0 ka \Rightarrow \omega_k \to 0 \text{ as } k \to 0.$$

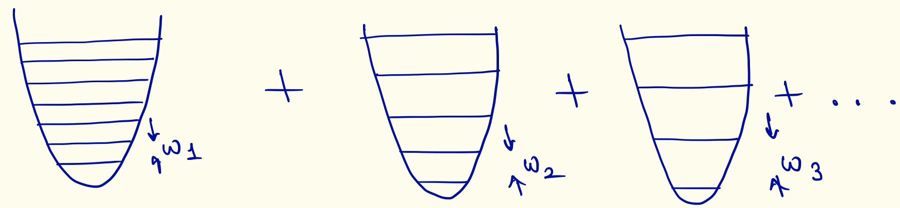
This is a universal feature of Goldstone modes irrespective of details of the Hamiltonian. For example, one may add a next-nearest neighbour interaction between the masses, or even add anharmonic terms. The modes will continue to vanish as $\omega \sim k$ as $k \to 0$. This non-trivial fact goes by the name of 'Universality'. That is, some features of a system are <u>insensitive</u> to microscopic details.

Having decomposed the modes into sum of decoupled harmonic oscillators, we can now use our standard technology of a, a^+ operators. Thus,

$$a_k = \sqrt{\frac{m\omega_k}{2}}\left[\hat{x}_k + i\frac{\hat{p}_k}{m\omega_k}\right]$$

$$H = \sum_k \omega_k \left(a^+_k a_k + \tfrac{1}{2}\right)$$

where $[a_k, a^+_{k'}] = \delta_{kk'}$.

$H =$ 

Since each harmonic oscillator mode can have an arbitrary number of excitations, the system is equivalent to a bosonic system with single-particle dispersion:

$$\boxed{\epsilon_k = \omega_k}$$

Thermodynamics:

$$Z = \mathrm{Tr}\, e^{-\beta \omega_k a^\dagger_k a_k}$$ [dropping zero-point energy]

$$= \prod_k \left[\frac{1}{1 - e^{-\beta\omega_k}} \right]$$

$$F = T \sum_k \log\left[1 - e^{-\beta\omega_k}\right]$$

$$\langle E \rangle = \partial_\beta [\beta F]$$

$$= \partial_\beta \left[\sum_k \log\left[1 - e^{-\beta\omega_k}\right] \right]$$

$$= \sum_k \frac{e^{-\beta\omega_k}\, \omega_k}{\left[1 - e^{-\beta\omega_k}\right]}$$

$$= \sum_k \frac{\omega_k}{\left[e^{\beta\omega_k} - 1\right]}$$

$$= \sum_k \omega_k \langle n_k \rangle$$

where $\langle n_k \rangle = \dfrac{1}{e^{\beta\omega_k} - 1}$ = average occupation number of the k'th mode.

For simplicity, let's restrict ourselves to temperatures $T \ll \hbar\omega_0$, so that one may work with the approximation,

$$\omega_k = \omega_0 k a \equiv c k$$

(c = sound velocity).

The average energy of the system is given by:

$$E = \sum_{\vec{k}} \frac{\hbar \omega_k}{e^{\beta \hbar \omega_k} - 1}$$

$$= \frac{N}{2\pi} \int \frac{\hbar c k \quad dk}{e^{\beta \hbar c k} - 1} \sim N T^2$$

(by scaling argument).

$$\Rightarrow \boxed{\frac{C_V}{N} \sim T}$$

(you can figure out the exact prefactor using $\int \frac{x^n}{e^x - 1} dx = \Gamma(n+1)\zeta(n+1)$ but that is a detail/ 'non-universal')

Generalization to 'd' space dimensions:

Naively in d-space dimensional cubic lattice:

$$E \overset{?}{=} \frac{V}{(2\pi)^d} \int \frac{d^d k}{e^{\beta \hbar c k} - 1} .$$

But this misses something important. Since sound modes (=Goldstone modes) have a direction of propagation, there are d independent ways to vibrate for a given $\vec{k}$ vector:

- 1 way to oscillate along the direction of propagation. (longitudinal sound mode)
- d−1 ways to oscillate perpendicular to the direction of propagation. (transverse sound modes)

Contrast this with the case of light (photon) where only transverse modes exist
- the two polarization choices in the previous lecture were exactly to account for that.

Even more, there is no symmetry reason for the longitudinal sound velocity c_l to be same as the transverse sound velocity c_t.

Thus,

$$E = E_t + E_l \qquad (T \ll \hbar\omega_0)$$

$$= \frac{V(d-1)}{(2\pi)^3}\int \frac{d^dk \;\; \hbar c_t k}{e^{\beta c_t \hbar k} - 1}$$

$$+ \frac{V}{(2\pi)^3}\int \frac{d^dk \;\; \hbar c_l k}{e^{\beta c_l \hbar k} - 1}$$

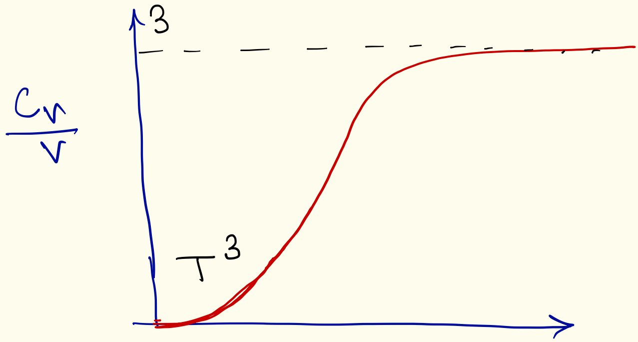
$$\Rightarrow \frac{E}{V} \sim \left[\frac{(d-1)}{c_t^d} + \frac{1}{c_l^d}\right] T^{d+1}$$

$$\boxed{\frac{C_V}{V} \sim \left[\frac{d-1}{c_t^d} + \frac{1}{c_l^d}\right] T^d}$$

In particular, when $d = 3$, $C_V \sim T^3$, a fact that is routinely observed in solids.

As one may expect, when $T \gg \hbar\omega_0$

$$\frac{C_V}{V} \rightarrow 3$$



Again, note the similarity between a sound mode ('phonon') and a light mode ('photon').