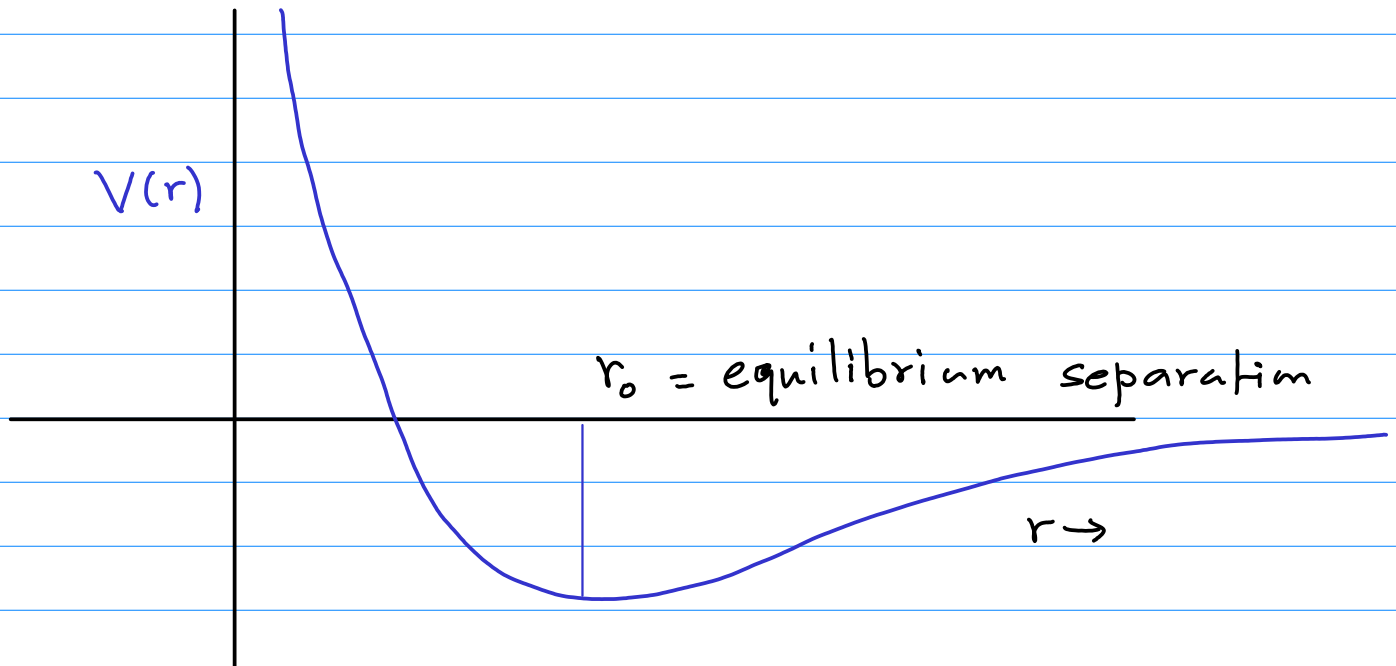# Many coupled oscillators

A diatomic molecule is the simplest realization of the harmonic oscillator in Nature. The potential between the two atoms, as a function of their separation, is

r_0 = equilibrium separation

One can expand V near r_0 ①

$$V(r) = V(r_0) + (r-r_0) \frac{dV}{dr}\Big|_{r_0} + \frac{1}{2}(r-r_0)^2 \frac{d^2V}{dr^2}\Big|_{r_0} + \cdots$$

Because r_0 is a minimum $\frac{dV}{dr}\Big|_{r_0} = 0$ ②

The Hamiltonian of the molecule is

$$\frac{\vec{P_1}^2}{2M_1} + \frac{\vec{P_2}^2}{2M_2} + \frac{1}{2}V_0''\left(|\vec{x}_1 - \vec{x}_2| - r_0\right)^2 \quad ③$$

This is a 1D oscillator (in the radial separation).

This is a little too hard to handle at the moment, because angular momentum, which we have not yet covered, is involved.

So let's turn to an easier problem. We take a ring of N identical atoms with periodic boundary conditions.

Let us assume that the force between nearest neighbors is harmonic, and that each atom can only move in 1D.

$$\mathcal{H} = \sum_{n=0}^{N-1} \left(\frac{P_n^2}{2M} + \frac{1}{2} M \omega_0^2 \left(X_{n+1} - X_n \right)^2 \right) \quad \text{④}$$

⑤

$$[X_n, P_{n'}] = i\hbar \, \delta_{nn'} \qquad [X_n, X_{n'}] = [P_n, P_{n'}] = 0$$

periodic b.c.
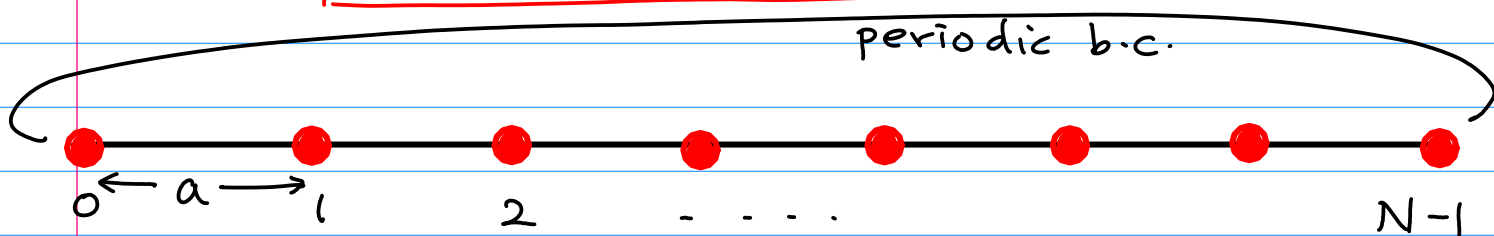
X_n is the deviation of the position of the atom at site n from its equilibrium position $\boxed{R_n = na}$ ⑥

We have N canonically conjugate pairs (X_n, P_n)

Since we have translation invariance we know we have to go to the plane wave basis.

Define $\tilde{\mathbb{X}}_k$ as

$$\mathbb{X}_n = \frac{1}{\sqrt{N}} \sum_{k=0}^{N-1} e^{i2\pi \frac{nk}{N}} \tilde{\mathbb{X}}_k \qquad ⑦$$

Now $\mathbb{X}_n$ is a hermitian operator, but $\tilde{\mathbb{X}}_k$ is not

$$\mathbb{X}_n^+ = \mathbb{X}_n \implies \boxed{\tilde{\mathbb{X}}_k^+ = \tilde{\mathbb{X}}_{-k}} \qquad ⑧$$

$-k \bmod N$ of course

Similarly

⑩

$$\mathbb{P}_n = \frac{1}{\sqrt{N}} \sum_{k=0}^{N-1} e^{2\pi i \frac{nk}{N}} \tilde{\mathbb{P}}_k \qquad ⑨$$

$$\boxed{\tilde{\mathbb{P}}_k^+ = \tilde{\mathbb{P}}_{-k}}$$

The inverse relations are

$$\tilde{\mathbb{X}}_k = \frac{1}{\sqrt{N}} \sum_{n=0}^{N-1} e^{-2\pi i \frac{nk}{N}} \mathbb{X}_n \qquad\qquad \tilde{\mathbb{P}}_k = \frac{1}{\sqrt{N}} \sum_{n=0}^{N-1} e^{-2\pi i \frac{nk}{N}} \mathbb{P}_n \qquad ⑪$$

Let's see what the commutators are.

$$[\tilde{\mathbb{X}}_k, \tilde{\mathbb{P}}_{k'}] = \frac{1}{N} \sum_{n=0}^{N-1} \sum_{n'=0}^{N-1} e^{-i2\frac{\pi}{N}(nk+n'k')} [\mathbb{X}_n, \mathbb{P}_{n'}]$$

⑫

$$= \frac{i\hbar}{N} \sum_{n=0}^{N-1} e^{-2\pi i \frac{n(k+k')}{N}} = i\hbar\, \delta_{k,-k'}$$

Let us pause for a minute here and think about what we have done.

Superficially, this looks very similar to the Fourier transform in the finite dimensional matrix Hamiltonians you did in your homeworks.

However, this is very different. There, we were taking linear combinations of states to go to a new basis. The demand was that the new basis be orthonormal.

Here, we are taking linear combinations of operators. The demand is that they still obey canonical commutation relations

There the Hilbert space was finite-dimensional

Here, even for a single Harmonic oscillator the Hilbert space is ∞-dimensional.

Now let's write the Hamiltonian in this basis.

$$\sum_{n=0}^{N-1} \mathbb{P}_n^2 = \frac{1}{N} \sum_{n=0}^{N-1} \sum_{k,k'=0}^{N-1} e^{\frac{2\pi i n}{N}(k+k')} \tilde{\mathbb{P}}_k \tilde{\mathbb{P}}_{k'}$$

$$= \sum_{k=0}^{N-1} \tilde{\mathbb{P}}_k \tilde{\mathbb{P}}_{-k}$$

(13)

$$\mathbb{X}_{n+1} - \mathbb{X}_n = \frac{1}{\sqrt{N}} \sum_{k=0}^{N-1} e^{\frac{2\pi i n k}{N}} \left(e^{\frac{2\pi i k}{N}} - 1 \right) \tilde{\mathbb{X}}_k$$

$$\sum_{n=0}^{N-1} (x_{n+1} - x_n)^2 = \frac{1}{N} \sum_{n=0}^{N-1} \sum_{k,k'=0}^{N-1} e^{\frac{2\pi i n}{N}(k+k')} \tilde{x}_k \tilde{x}_{k'} \left(e^{\frac{2\pi i k}{N}} - 1\right) \otimes \left(e^{\frac{2\pi i k'}{N}} - 1\right)$$

$$= \sum_{k=0}^{N-1} \tilde{x}_k \tilde{x}_{-k} \left(2 - 2\cos\frac{2\pi k}{N}\right) \quad \text{(14)}$$

$$\mathcal{H} = \sum_{k=0}^{N-1} \left[\frac{\tilde{P}_k \tilde{P}_{-k}}{2M} + \frac{1}{2} M\omega_0^2 \left(2 - 2\cos\left(\frac{2\pi k}{N}\right)\right) \tilde{x}_k \tilde{x}_{-k}\right] \quad \text{(15)}$$

As expected, we have partially diagonalized the Hamiltonian. Only k and $-k \bmod N$ are coupled.

To go further let us decompose $\tilde{x}_k$, $\tilde{x}_{-k}$ $\tilde{P}_k$ and $\tilde{P}_{-k}$ as follows

$$\tilde{x}_k = \frac{Q_{1k} + i Q_{2k}}{\sqrt{2}} \qquad \tilde{x}_{-k} = \frac{Q_{1k} - i Q_{2k}}{\sqrt{2}} \qquad \text{(16)}$$

$$Q_{ik}^+ = Q_{ik}$$
$$\Pi_{ik}^+ = \Pi_{ik}$$

$$\tilde{P}_k = \frac{\Pi_{1k} - i\Pi_{2k}}{\sqrt{2}} \qquad \tilde{P}_{-k} = \frac{\Pi_{1k} + i\Pi_{2k}}{\sqrt{2}}$$

The $\frac{1}{\sqrt{2}}$ factors and the arrangement of factors of i is intended to make Q_{1k}, Π_{1k} and Q_{2k}, Π_{2k} canonical pairs.

$$\left[Q_{ik}, Q_{jk'}\right] = 0 = \left[\Pi_{ik}, \Pi_{jk'}\right]$$

$$\left[Q_{ik}, \Pi_{jk'}\right] = i\hbar \, \delta_{ij} \, \delta_{kk'} \quad \text{(17)}$$

$k=0$ has to be treated specially, because

$$\tilde{\mathbb{X}}_0^+ = \tilde{\mathbb{X}}_0 \qquad \text{and} \qquad \tilde{\mathbb{P}}_0^+ = \tilde{\mathbb{P}}_0 \qquad \text{(18)}$$

Another potential special value is if

$$-k = k \bmod N \qquad \text{which means}$$
$$k = \frac{N}{2} \qquad \text{and} \qquad N \text{ even.}$$

Let us avoid this possibility by making N odd. Now only $k=0$ is special.

$$\tilde{\mathbb{X}}_0 \equiv \mathbb{Q}_0 \qquad\qquad \tilde{\mathbb{P}}_0 = \Pi_0 \qquad\qquad \text{(19)}$$

$$\mathbb{Q}_0^+ = \mathbb{Q}_0 \quad, \quad \Pi_0^+ = \Pi_0 \qquad\qquad [\mathbb{Q}_0, \Pi_0] = i\hbar$$

Note that for $k=0$ $\quad 2 - 2\cos\frac{2\pi k}{N} = 0$

Since $\quad -k = N-k \bmod N \quad$ we see that for $k \neq 0$ only $\quad k = 1, \cdots \frac{N-1}{2}$ $\quad$ (N odd) are independent.

For each such k we have two pairs of canonically conjugate variables $(\mathbb{Q}_{1k}, \Pi_{1k}), (\mathbb{Q}_{2k}, \Pi_{2k})$ $\Rightarrow$ $2\left(\frac{N-1}{2}\right) = N-1$. Finally for $k=0$ we have

one pair, which brings the total number of canonical pairs to N, as expected.

$\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad$ (20)

Let us define $\qquad\qquad \boxed{\theta_k = \frac{2\pi k}{N} \qquad 1 - \cos\theta_k = 2\sin^2\frac{\theta_k}{2}}$

$$\mathcal{H} = \frac{\Pi_0^2}{2M} + \sum_{k=1}^{\frac{N-1}{2}} \frac{(\Pi_{1k}^2 + \Pi_{2k}^2)}{2M} + \frac{M}{2}\left(2\omega_0 \sin\frac{\theta_k}{2}\right)^2 (Q_{1k}^2 + Q_{2k}^2) \qquad (21)$$

Now these are decoupled Harmonic oscillators. Let us go to their ladder operators. The natural length is

$$\ell_k = \sqrt{\frac{\hbar}{2M\omega_0 \sin\theta_{k/2}}} \qquad\qquad \omega_k = 2\omega_0 \sin\frac{\theta_k}{2} \quad (22)$$

$$a_{ik} = \frac{1}{\sqrt{2}}\left\{ \sqrt{\frac{2M\omega_0 \sin\theta_{k/2}}{\hbar}}\, Q_{ik} + \frac{i\,\Pi_{ik}}{\sqrt{2M\omega_0 \hbar \sin\frac{\theta_k}{2}}} \right\} \qquad (23)$$

$$a_{ik}^{+} = \frac{1}{\sqrt{2}}\left\{ \sqrt{\frac{2M\omega_0 \sin\theta_{k/2}}{\hbar}}\, Q_{ik} - \frac{i\,\Pi_{ik}}{\sqrt{2M\omega_0 \hbar \sin\frac{\theta_k}{2}}} \right\}$$

$$\mathcal{H} = \frac{\Pi_0^2}{2M} + \sum_{k=1}^{\frac{N-1}{2}} \hbar\omega_k \left[a_{1k}^{+}a_{1k} + \frac{1}{2} + a_{2k}^{+}a_{2k} + \frac{1}{2} \right] \qquad (24)$$

The mode at $k=0$ is not an oscillator, because there is no restoring force. Instead it corresponds to the center-of-mass motion of the atoms in the ring.

The $k \neq 0$ modes are quantized lattice vibrations called phonons. They have a dispersion (the relation between ω & k)
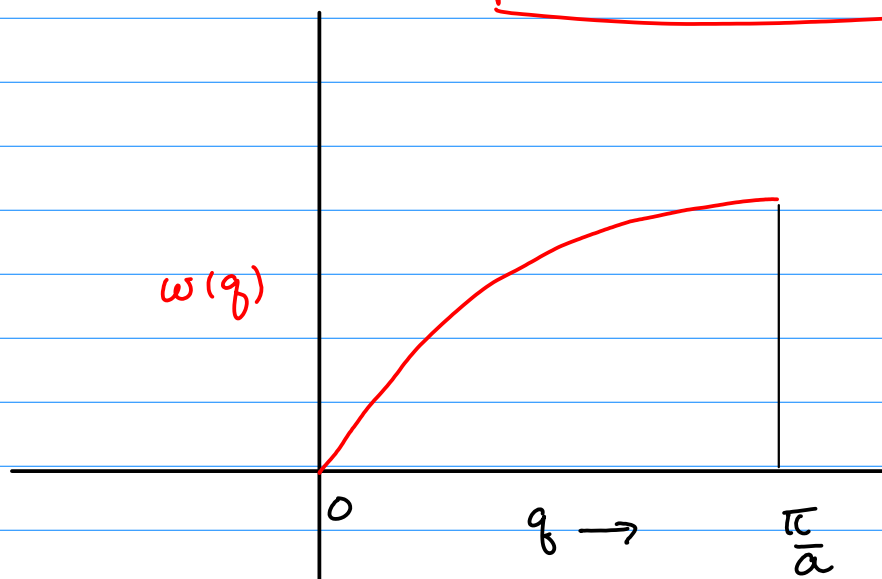
$$\omega_k = 2\omega_0 \sin\frac{\pi k}{N}$$

In the limit when N becomes very large we get a quasicontinuous spectrum

If we plot $\boxed{\dfrac{2\pi k}{N} = \theta_k \equiv qa}$ (25)

a = equilibrium spacing of atoms

$\omega(q)$

0 $q \rightarrow$ $\dfrac{\pi}{a}$

linearly dispersing modes are called **acoustic modes** because they transmit sound

An interesting quantity to compute is the Δx of a particular atom, say the one at $n=0$ when the system of oscillators is in its ground state.

The eigenstates are labelled by nonnegative integers n_{1k}, n_{2k}, for $k \in [0, \frac{N-1}{2}]$.

(26)

$$H\,|\{n_{1k}, n_{2k}\}\rangle = \sum_{k=0}^{\frac{N-1}{2}} \left\{ \hbar\omega_k \left(n_{1k} + n_{2k} + 1\right)\right\} |\{n_{1k}, n_{2k}\}\rangle$$

The ground state is $n_{1k} = n_{2k} = 0 \ \forall k$ $|gs\rangle$

From (7)

$$x_0 = \frac{1}{\sqrt{N}} \sum_{k=0}^{N-1} \tilde{x}_k$$ (27)

So $\quad$ $\boxed{\langle gs| \tilde{x}_0^2 |gs\rangle = \dfrac{1}{N} \displaystyle\sum_{k=0}^{N-1} \sum_{k'=0}^{N-1} \langle gs| \tilde{\tilde{x}}_k \tilde{\tilde{x}}_{k'} |gs\rangle}$ $\quad$ (28)

From (16) we know that only $\langle gs| \tilde{\tilde{x}}_k \tilde{\tilde{x}}_{-k} |gs\rangle$ will be nonzero.

$\boxed{\langle \tilde{x}_0^2 \rangle = \dfrac{2}{N} \displaystyle\sum_{k=1}^{\frac{N-1}{2}} \langle Q_{1k}^2 + Q_{2k}^2 \rangle}$ $\quad$ (29)

Ignore $k=0$ because CM fixed.

For a single oscillator we know $\boxed{\langle Q^2 \rangle = \dfrac{\ell^2}{2}}$ $\quad$ (30)

So $\quad$ $\boxed{\langle \tilde{x}_0^2 \rangle = \dfrac{2}{N} \displaystyle\sum_{k=1}^{\frac{N-1}{2}} \dfrac{\hbar}{2M\omega_0 \sin\frac{\theta_k}{2}}}$ $\quad$ (31) $\quad$ $\theta_k = \dfrac{2\pi k}{N}$

In the $N \to \infty$ limit

$\boxed{\langle \tilde{x}_0^2 \rangle = \dfrac{\hbar}{M\omega_0} \displaystyle\int_0^\pi \dfrac{d\theta}{2\pi} \cdot \dfrac{1}{\sin(\theta/2)}}$ $\quad$ (32) $\quad$ diverges!!

Quantum fluctuations make a 1D solid unstable!

When one goes to 2D there are two integers k_1 and k_2 representing plane waves propagating along x and y.

Now the analog of $\quad$ is

$\boxed{\langle \vec{x}_0^2 \rangle = \dfrac{\hbar}{M\omega_0} \displaystyle\int_0^\pi \dfrac{d\theta_x \, d\theta_y}{\sqrt{\sin^2\frac{\theta_x}{2} + \sin^2\frac{\theta_y}{2}}}}$ $\quad$ (33)

This converges, making 2D lattices stable at $T=0$.

Let's do a bit of thermodynamics.

Imagine that one constructs a classical solid of N atoms (you cannot do this, but let's imagine we can). We imagine that atoms are interacting with each other harmonically (like particles connected by springs)
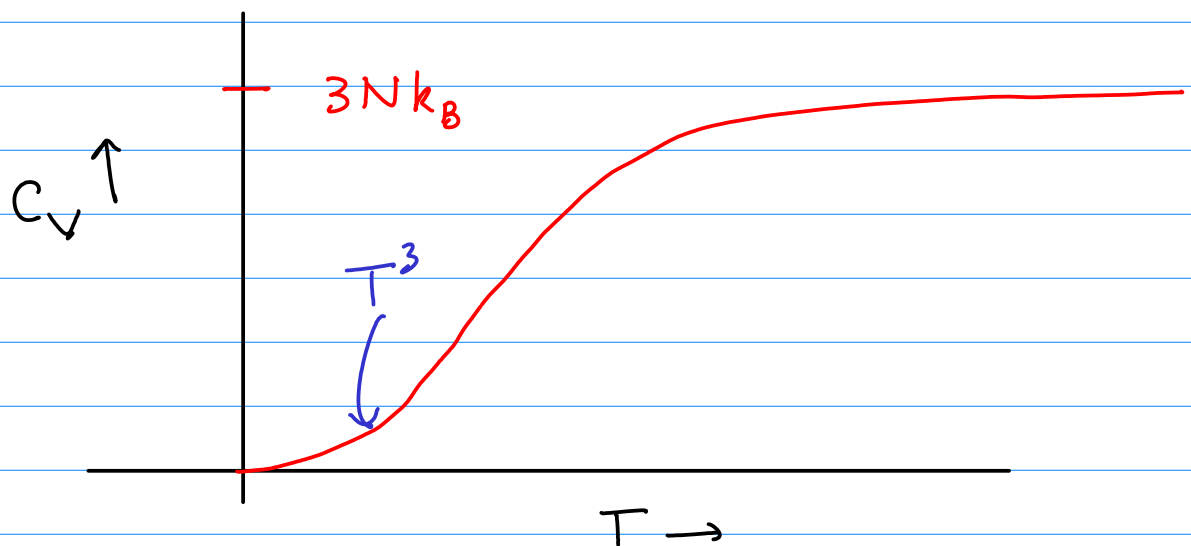
Classically, each mode has energy $k_B T/2$
Since each particle has 3 directions to move and potential as well as kinetic energy

$$U = 3 N k_B T$$ (34)

=) Classical Specific heat is

$$C_V = 3 N k_B$$ (35)   Independent of T!

Experiments by Nernst and others showed the following qualitative behavior

$3Nk_B$

C_V ↑

T^3

$T \rightarrow$

The first attempt to tackle this quantum mechanically was by Einstein in 1907. He assumed that all the interactions between atoms could be represented by quantum oscillators of frequency ω_0

For a single oscillator

$$E_n = \hbar \omega_0 (n + 1/2)$$

The partition function is the sum of Boltzmann weights

$$z = \sum_{n=0}^{\infty} e^{-\beta E_n} \quad (36)$$

$$\beta = \frac{1}{k_B T}$$

↗ Boltzmann's constant.

$$z = e^{-\beta \frac{\hbar \omega_0}{2}} \sum_{0}^{\infty} e^{-n\beta \hbar \omega_0}$$

$$= \frac{e^{-\beta \frac{\hbar \omega_0}{2}}}{1 - e^{-\beta \hbar \omega_0}} \quad (37)$$

For 3N identical and independent oscillators

$$Z_E = z^{3N} \quad (38)$$

E for Einstein

Now, in thermodynamics we define the Helmholz free energy F as

$$Z = e^{-\beta F} \implies F = -k_B T \ln Z \quad \text{(39)}$$

$$F_E = -3Nk_B T \left\{ -\beta \frac{\hbar \omega_0}{2} - \ln\left(1 - e^{-\beta \hbar \omega_0}\right) \right\}$$

$$F_E = \frac{3N\hbar \omega_0}{2} + 3Nk_B T \ln\left(1 - e^{-\beta \hbar \omega_0}\right) \quad \text{(40)}$$

Recall that F, the internal energy U and the entropy S are all state functions

$$dU = TdS - PdV \quad \text{(41)}$$

P = pressure

V = volume

$$\text{(42)} \quad F = U - TS$$

Legendre transform

$$\implies dF = TdS - PdV - TdS - SdT$$

$$dF = -SdT - PdV \quad \text{(43)}$$

$$\implies \quad S = -\left(\frac{\partial F}{\partial T}\right)_V \quad \text{(44)}$$

Since TdS is the amount of heat supplied under quasistatic conditions, the specific heat at constant volume is

$$C_V = T\left(\frac{\partial S}{\partial T}\right)_V = -T\left(\frac{\partial^2 F}{\partial T^2}\right)_V \quad \text{(45)}$$

Let's apply this to Einstein's model

$$S_E = -\left(\frac{\partial F_E}{\partial T}\right)_V = 3Nk_B \ln\left(1-e^{-\beta\hbar\omega_0}\right)$$

$$+ 3Nk_B T \frac{e^{-\beta\hbar\omega_0}}{1-e^{-\beta\hbar\omega_0}} \frac{\hbar\omega_0}{k_B T^2}$$

$$\boxed{S_E = 3Nk_B \ln\left(1-e^{-\beta\hbar\omega_0}\right) + \frac{3N\hbar\omega_0}{T} \frac{1}{e^{\beta\hbar\omega_0}-1}} \quad \text{(46)}$$

$$C_{V,E} = T\left(\frac{\partial S}{\partial T}\right)_V = T\left\{3Nk_B \frac{e^{-\beta\hbar\omega_0}}{1-e^{-\beta\hbar\omega_0}} \frac{\hbar\omega_0}{k_B T^2} - \frac{3N\hbar\omega_0}{T^2}\frac{1}{(e^{\beta\hbar\omega_0}-1)}\right.$$

$$\left. + 3N\frac{\hbar\omega_0}{T} \frac{e^{\beta\hbar\omega_0}}{(e^{\beta\hbar\omega_0}-1)^2} \frac{\hbar\omega_0}{k_B T^2}\right\}$$
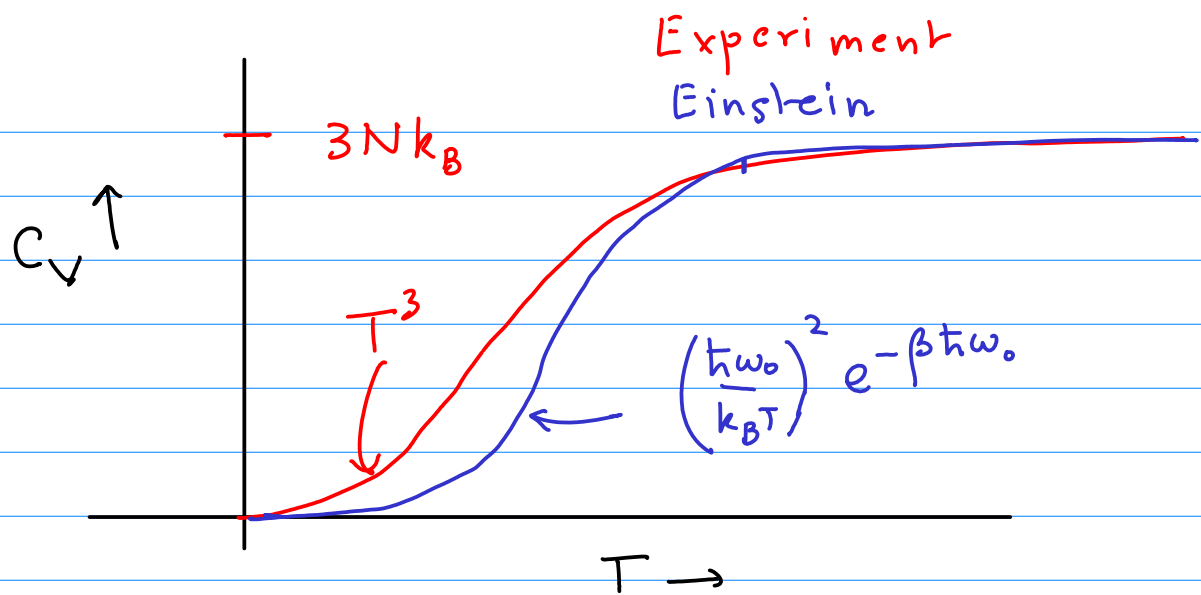
$$\boxed{C_{V,E} = 3Nk_B \left(\frac{\hbar\omega_0}{k_B T}\right)^2 \frac{e^{\beta\hbar\omega_0}}{(e^{\beta\hbar\omega_0}-1)^2}} \quad \text{(47)}$$

As $T\to\infty$ $\beta\to 0$ and this reduces to $3Nk_B$, which is the classical result

As $T\to 0$ $\beta\to\infty$ and this behaves like

$$\boxed{3Nk_B\left(\frac{\hbar\omega_0}{k_B T}\right)^2 e^{-\frac{\hbar\omega_0}{k_B T}} \to 0} \quad \text{(48)}$$

The qualitative plot is shown below

The graph shows C_V on the vertical axis and T on the horizontal axis, with a dashed line at $3Nk_B$. Labels: "Experiment" (red curve), "Einstein" (blue curve), T^3 pointing to low-temperature region, and $\left(\frac{\hbar\omega_0}{k_B T}\right)^2 e^{-\beta\hbar\omega_0}$ labeling the Einstein curve.

While this is a huge improvement on the classical result, it is not quite right at low temperature.

Debye (1912) realized what was needed to get the correct low-T behavior.

The key point is that the energies of the oscillators are not all equal.

The low-energy oscillators play the most important role at low T. In a solid these are the acoustic modes.

There are 3 acoustic modes in any 3D solid. Each mode is labelled by 3 angles $\theta_x, \theta_y, \theta_z$. Let us, for simplicity take them to all have the same energy dispersion

$$\omega(\vec{\theta}) = 2\omega_0 \sqrt{\sin^2\frac{\theta_x}{2} + \sin^2\frac{\theta_y}{2} + \sin^2\frac{\theta_z}{2}} \qquad \text{(49)}$$

$$\approx \omega_0 \sqrt{\theta_x^2 + \theta_y^2 + \theta_z^2} \qquad \text{at small } |\vec{\theta}|.$$

The free energy of this set of oscillators is

$$F = k_B T \sum_{k_x, k_y, k_z} \left\{ \frac{\hbar\omega(\vec{k})}{k_B T} + \ln\left(1 - e^{-\beta\hbar\omega(\vec{k})}\right) \right\} \qquad \text{(50)}$$

a = lattice spacing

Recall

$$\sum_{k_x, k_y, k_z} \rightarrow \frac{V}{a^3} \int \frac{d\theta_x \, d\theta_y \, d\theta_z}{(2\pi)^3} \qquad \text{(51)}$$

$$F = 3\frac{V}{a^3} \int \frac{d\theta_x \, d\theta_y \, d\theta_z}{(2\pi)^3} \left\{ \hbar\omega(\vec{\theta}) + k_B T \ln\left(1 - e^{-\beta\hbar\omega(\vec{\theta})}\right) \right\} \qquad \text{(52)}$$

3 acoustic modes

$$S = -\frac{\partial F}{\partial T} = 3\frac{V}{a^3} \int \frac{d^3\theta}{(2\pi)^3} \left\{ k_B \ln\left(1 - e^{-\beta\hbar\omega(\vec{\theta})}\right) \right.$$
$$\left. + k_B T \frac{e^{-\beta\hbar\omega(\vec{\theta})}}{1 - e^{-\beta\hbar\omega(\vec{\theta})}} \hbar\omega(\vec{\theta}) \frac{1}{k_B T^2} \right\}$$

$$S = 3\frac{V}{a^3} \int \frac{d^3\theta}{(2\pi)^3} \left\{ k_B \ln\left(1 - e^{-\beta\hbar\omega(\vec{\theta})}\right) + \frac{\hbar\omega(\vec{\theta})}{T} \frac{1}{e^{\beta\hbar\omega(\vec{\theta})} - 1} \right\} \qquad \text{(53)}$$

Some terms cancel when we take $\frac{\partial S}{\partial T}$

$$\frac{\partial S}{\partial T} = \frac{3V}{a^3} \int_0^\pi \frac{d^3\theta}{(2\pi)^3} \frac{(\hbar\omega(\bar{\theta}))^2 \, e^{\beta\hbar\omega(\bar{\theta})}}{k_B T^3 \, (e^{\beta\hbar\omega(\bar{\theta})}-1)^2} \qquad (54)$$

So the specific heat is (55)

$$C_V = T\frac{\partial S}{\partial T} = \frac{3}{k_B T^2} \frac{V}{a^3} \int \frac{d^3\theta}{(2\pi)^3} \frac{(\hbar\omega(\bar{\theta}))^2 \, e^{\beta\hbar\omega(\bar{\theta})}}{(e^{\beta\hbar\omega(\bar{\theta})}-1)^2}$$

At low temperature $k_B T \ll \hbar\omega_0$ only low-energy modes are thermally populated. In this case we can say

$$\boxed{\omega(\bar{\theta}) \approx \omega_0 |\bar{\theta}|} \qquad (56)$$

and go to

spherical polar coordinates in $\bar{\theta}$. Do the angular integrals.

$$C_V \approx \frac{3}{k_B T^2} \frac{V}{a^3} \frac{4\pi}{(2\pi)^3} \int_0^\pi \theta^2 d\theta \frac{(\hbar\omega_0)^2 \theta^2 \, e^{\beta\hbar\omega_0\theta}}{(e^{\beta\hbar\omega_0\theta}-1)^2}$$

Define $\boxed{\beta\hbar\omega_0\theta = \xi \qquad d\theta = \frac{d\xi}{\beta\hbar\omega_0}} \qquad (57)$

$$C_V \simeq \frac{3}{k_B T^2} \frac{V}{a^3} \frac{4\pi}{(2\pi)^3} (\hbar\omega_0)^2 \frac{1}{(\beta\hbar\omega_0)^5} \int_0^{\beta\hbar\omega_0\pi} d\xi \frac{\xi^4 \, e^{\xi}}{(e^{\xi}-1)^2} \qquad (58)$$

when $\hbar\omega_0 \gg k_B T$ $\quad \beta\hbar\omega_0\pi \gg 1$. The integral converges rapidly beyond $\xi \approx 5$ so

we can replace the upper limit by ∞ with negligible error.

$$C_V \simeq k_B \cdot \frac{3}{2\pi^2} \frac{V}{q^3} \left(\frac{k_B T}{\hbar \omega_0}\right)^3 \int_0^{\infty} d\xi \frac{\xi^4 e^{\xi}}{(e^{\xi}-1)^2}$$ (59)

So, in any 3D solid, the specific heat should go as T^3 at low temperature

In a complex solid, in addition to acoustic modes, there are usually also "optical" modes, which have $\omega(\bar{\theta}) > 0$ for all $\bar{\theta}$. The calculation can become very complicated.

However, the fact that at low T the specific heat goes as T^3 while at high T it saturates at $3Nk_B$ is universal.