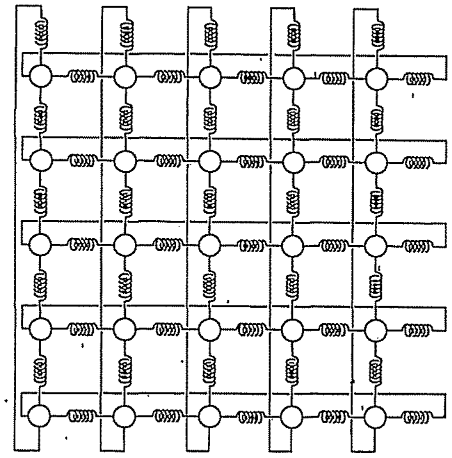
Appendix C

Physicist's View of Collective Excitations

(C1)



T=0 Ground State

Ordinary People's View

Many atoms / Many bonds
Nothing is vibrating

Ground State

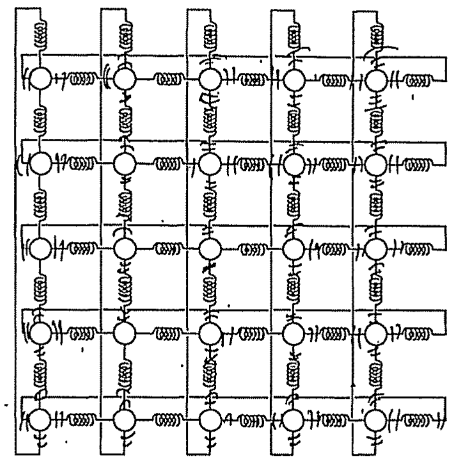
* No excited oscillators
for all independent oscillators characterized by $\omega_s(\vec{q})$

i.e. $n_{s,\vec{q}} = 0$
{ for all branches s
and all $\vec{q}$ in 1st B.Z.
all modes!

Physicist's Point of View
(Simple!)
[No phonons!]

(C2)

$T \neq 0$



Ordinary people's view

Many Atoms Vibrating!

Low-energy excitations

Some phonons

$$\langle n_{s,\vec{q}} \rangle = \frac{1}{e^{\hbar\omega_s(\vec{q})/kT} - 1}$$

Excitations of the independent oscillators

$\langle n_{s,\vec{q}} \rangle$ phonons, each with energy $\hbar\omega_s(\vec{q})$ and "momentum" $\hbar\vec{q}$

Note: $\langle n_{s,\vec{q}} \rangle$ depends on $\hbar\omega_s(\vec{q})$ and kT.

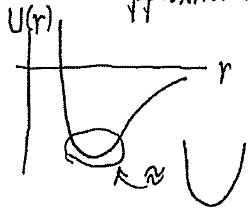
This simple picture makes calculations easier. For example, one can write down the energy of the system at temperature T as:

$$U(T) = \underbrace{\sum_{\substack{\text{all branches} \\ s}} \sum_{\substack{\text{all } \vec{q} \\ \text{in } 1^{st}\text{BZ}}}}_{\substack{\text{sum over} \\ \text{all modes}}} \underbrace{\hbar\omega_s(\vec{q})}_{\substack{\text{energy of each} \\ \text{excitation of the} \\ \text{mode } \omega_s(\vec{q})}} \cdot \underbrace{\frac{1}{e^{\hbar\omega_s(\vec{q})/kT} - 1}}_{\substack{\text{excitation of the} \\ \text{mode } \omega_s(\vec{q})}} + \underbrace{\text{Zero Point energy}}_{\text{Just a constant}}$$

- This sum can be carried out by using the density of modes $D(\omega)d\omega$.
- Heat capacity $\frac{\partial U}{\partial T} = C_v$

- Thus, the lattice vibrations at $T \neq 0$ are described as the existence of some phonons.
- There are electrons in the solid. The electrons will be affected by lattice vibrations. In terms of phonons, there are <u>electron-phonon interactions</u>. This is a reason for having <u>resistance</u>.
- <u>How about phonon-phonon interactions</u>?

Harmonic Approximation $\Rightarrow$ Decoupled independent oscillators



$\Downarrow$

phonons are independent non-interacting excitations

$\Downarrow$

no phonon-phonon interactions

<u>Beyond</u> Harmonic Approximation $\Rightarrow$ $\underbrace{\text{Harmonic Approximation}}_{\text{independent phonons}} + \underbrace{\text{Correction terms}}_{\substack{\text{phonon-phonon} \\ \text{interactions due to} \\ \text{anharmonic corrections.}}}$