

Lecture on Solid State

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1 First Lecture

In this lecture we are going to discuss the early state of solid state physics. At first let us recall the description of Heat capacity in a volume:

$$C_v = \left. \frac{\partial u}{\partial T} \right|_V \quad (1)$$

In reality the heat constant is made of two parts:

$$C_v = C_{\text{elec}} + C_{\text{lattice}} \quad (2)$$

The lattice is the network of nucleuses, in this section we are going to look into the lattice part. The energy of the lattice is described as below:

$$u_{\text{lattice}} = \sum_k \sum_p u_{kp} \quad (3)$$

where k is the network properties and p is the polarization. Assuming that there exists a wave in the lattice there is a graph for possible ω in a $k = \frac{2\pi}{\lambda}$ since the wave can be longitudinal and transverse we can have polarizations.

In our simplest models we can write the equation for energy as a collection of simple harmonic oscillator:

$$u_{\text{lattice}} = \sum_{k,p} \langle n_{k,p} \rangle \hbar \omega_{k,p} \quad (4)$$

$n_{k,p}$ is the average heat number of occupation, meaning that in temperature T how many heat equilibrium do we have. and $\hbar \omega_{k,p}$ is the energy of oscillation with momentum k and polarization p . calculation of occupation number is to be left for later but the answer is of the form:

$$\langle n \rangle = \frac{1}{e^{\hbar \omega / k_B T} - 1} \quad (5)$$

therefore the energy would be:

$$u = \sum_{k,p} \frac{\hbar \omega_{k,p}}{e^{\beta \hbar \omega_{k,p}} - 1} \quad (6)$$

If the number of nodes in the lattice is big enough we can transform the summation into integral with a transformation multiplication:

$$\int d_k \frac{dk}{d\omega} d\omega \quad (7)$$

So the work is to find d_k . This is also equivalent with writing:

$$\int D_p(\omega) d\omega \quad (8)$$

Here $D(\omega)$ the phonon density of state, therefore we write:

$$u = \sum_p \int d\omega D_p(\omega) \frac{\hbar \omega}{e^{\frac{\hbar \omega}{k_B T}} - 1} \quad (9)$$

Then we have the heat capacity of lattice as:

$$C_{\text{lattice}} \equiv \frac{\partial u}{\partial T} = k_B \sum_p \int_0^\infty d\omega D(\omega) \frac{x^2 e^x}{(e^x - 1)^2} \quad (10)$$

where $x = \frac{\hbar \omega}{k_B T}$. Now let us find the phonon density let us write again:

$$D(\omega) d\omega = d_k \frac{dk}{d\omega} d\omega \quad (11)$$

We would use the periodic boundary conditions, which means that:

$$u(x) = u(x + L) \quad (12)$$

Since the lattice has a reoccurring shape this is a good boundary condition for first investigation. For this to happen the first thing we can write is of the form:

$$u_0 e^{kx - \omega t} = u_0 e^{k(x+L) - \omega t} \quad (13)$$

This means simply:

$$k = \frac{2\pi}{L} n \quad (14)$$

here n is $0, \pm 1, \pm 2, \dots, \pm N$ where N is the number of cells. One can find the allowed k s of k -space (here 1 dimensional) with:

$$\text{Number of allowed } k \equiv \frac{\text{Volume of } k}{\text{Distance of nodes}} = \frac{K}{\frac{2\pi}{L}} \quad (15)$$

We can easily write this for a 3 dimensional lattice, by just having:

$$u(\vec{x}) = u(\vec{x} + \vec{L}) \quad (16)$$

and for three dimensions the number of allowed k are:

$$N_k = \frac{\frac{4}{3}\pi k^3}{\left(\frac{2\pi}{L_x}\right)\left(\frac{2\pi}{L_y}\right)\left(\frac{2\pi}{L_z}\right)} = \frac{\frac{4}{3}\pi k^3}{\frac{8\pi}{V}} \quad (17)$$

It is obvious that since the number of modes with a polarization p between ω and $\omega + d\omega$ is as follows:

$$D(\omega) d\omega \quad (18)$$

leading to the formula:

$$D(\omega) = \frac{dN}{d\omega} \rightarrow dN = d\omega D(\omega) \quad (19)$$

Thus we can write :

$$D(\omega) = \frac{dN}{d\omega} \quad (20)$$

$$= \frac{dN}{dk} \frac{dk}{d\omega} \quad (21)$$

$$= \frac{4\pi k^2}{\left(\frac{2\pi}{L}\right)^3} \frac{dk}{d\omega} \quad (22)$$

$$D(\omega) = \frac{V k^2}{2\pi^2} \frac{dk}{d\omega} \quad (23)$$

to have $dk/d\omega$ we have to use approximation: 1. Debye approximation 2. Einsteins approximation.

1.1 Debay Approximation

debay noticed that The first third Dispersion Curve can be approximated linearly:

$$\omega \propto k \quad (24)$$

$$\omega = v k \quad (25)$$

therefore $\frac{dk}{d\omega} = \frac{1}{v}$, and we can find the phonon density:

$$D(\omega) = \frac{V k^2}{2\pi^2} \frac{1}{v} \quad (26)$$

since this is an approximation we don't go over all k s, instead we would go until a known k called debay's k , or k_D . therefor ethe number of all modes would be:

$$N = \frac{\frac{4}{3}\pi k_D^3}{(2\pi)^3/V} \quad (27)$$

And the energy would become:

$$u = \int d\omega D(\omega) \langle n(\omega) \rangle \hbar\omega = \int_0^{\omega_D} d\omega \left(\frac{V\omega^2}{2\pi^2 v^3} \right) \frac{\hbar\omega}{e^{\beta\hbar\omega} - 1} \quad (28)$$