Condensed Matter Physics – FK7060, Feb. 13, 2018.

Lecture 10 – Lattice vibrations II

Reading

Ashcroft & Mermin, Ch. 23

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- Normal modes
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- Zero-point vibrations
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Central concepts

- **Normal modes**

  A general motion of N ions is represented as a superposition (linear combination) of $3N$ *normal modes* of vibration, each with its own characteristic frequency.

  The allowed energies of an oscillator with frequency ν are given by

  $$\left(n + \frac{1}{2}\right) h\nu, \qquad n = 0, 1, 2, \ldots \qquad (h\nu = \hbar\omega)$$

  The $3N$ normal modes correspond to $3N$ oscillators, each with the above possible energies.

  If the crystal has a primitive cell of p ions, there are $3p$ branches, each with $N_{cell} = N/p$ normal modes.

- **Phonons**

  Instead of talking about the nth energy state of a certain normal mode of branch s and wave vector $\mathbf{K}$, one says that there is n phonons of type s with wave vector $\mathbf{K}$ present in the crystal.

  The number of phonons in each mode at thermal equilibrium is given by the Bose-Einstein distribution

  $$n_s(\mathbf{K}) = \frac{1}{e^{\hbar\omega_s(\mathbf{K})/k_B T} - 1}$$

- **Zero-point vibrations**

  Summing the energy of all oscillators gives a contribution

  $$u_0 = \frac{1}{V} \sum_{\mathbf{K}s} \frac{1}{2} \hbar\omega_s(\mathbf{K})$$

  to the energy density. This vibration energy of $\hbar\omega_s(\mathbf{K})/2$ per mode is present even at $T = 0$.

- **High-temperature specific heat**

  The temperature dependent part of the energy density of a harmonic crystal is given by summing the number of phonons $n_s(\mathbf{K})$ times their energy $\hbar\omega_s(\mathbf{K})$,

$$u = \frac{1}{V}\sum_{\mathbf{K}s}\frac{\hbar\omega_s(\mathbf{K})}{e^{\hbar\omega_s(\mathbf{K})/k_BT}-1}$$

  At high temperatures $e^x \approx 1 + x$, so that $n_s = k_BT/\hbar\omega$. Then the expression becomes a sum over k_BT, so that $u \approx 3nk_BT$ $(n = N/V)$. This gives the classical Dulong-Petit specific heat

$$c_v = \frac{\partial u}{\partial T} = 3nk_B$$

  Anharmonic effects are the main reason for deviations at high T from this value.

- **Debye model**

  The Debye model makes two assumptions

  ⋆ $\omega = v_s|K|$, where v_s is the sound velocity

  ⋆ Introduce $\omega_D = v_sK_D$ such that a sphere of radius K_D contains N_{ion} allowed wave vectors (corresponding to $3N$ states in 3D with three polarization directions).

  Since the (reciprocal) volume per $\mathbf{K}$-point is $(2\pi)^3/V$, the second assumption gives

$$K_D = (6\pi^2 n)^{1/3}$$

  where $n = N/V$.

- **Debye temperature**

  The Debye temperature Θ_D is defined from

$$\hbar\omega_D = k_B\Theta_D$$

- **Low-temperature specific heat**

  Using the Debye model, letting

$$\sum_{\mathbf{K}} \rightarrow \frac{V}{(2\pi)^3}\int d\mathbf{K}$$

  and letting $d\mathbf{K} = 4\pi K^2 dK$, the heat capacity at low temperature can be written as

$$c_v \approx 234\left(\frac{T}{\Theta_D}\right)^3 nk_B$$

- **Einstein model**

  The Einstein model makes the assumption that all modes have the same frequency, i.e.,

$$\omega(\mathbf{K}) = \omega_E$$

  This assumption is thus best suited for the optical branches, where ω does not go to zero at long wavelengths (small K). Similarly to Θ_D an Einstein temperature Θ_E can be defined, $\hbar\omega_E = k_B\Theta_E$.

- **Density of normal modes**

  It is useful to introduce the density of normal modes $D(\omega)$ corresponding to the number of modes between ω and $\omega + d\omega$. As earlier, we define $g(\omega) = D(\omega)/V$.

With the Debye model, this gives

$$g_D(\omega)\mathrm{d}\omega = 3\frac{1}{(2\pi)^3}4\pi K^2\mathrm{d}K$$

i.e. (Eq. 23.36)

$$g_D(\omega) = \frac{3}{2\pi^2}\frac{\omega^2}{v_s^3}$$

for frequencies up to ω_D.

For the Einstein model, all modes have the same frequency ω_E so that

$$g_E(\omega) = n\delta(\omega - \omega_E)$$

where $\delta(x)$ is the Dirac delta function.

- **van Hove singularities**

  Just as for electrons, the density of states can be obtained as an integral over a constant-energy surface S,

$$g(\omega) = \sum_s \int \frac{\mathrm{d}S}{(2\pi)^3}\frac{1}{|\nabla\omega_s(\mathbf{K})|}$$

  Since $\nabla\omega_s(\mathbf{K})$ may become zero, the slope $\mathrm{d}g/\mathrm{d}\varepsilon$ displays singularities, also known as *van Hove singularities*.