# Physics 474 – Applied Solid State Physics - Course Notes

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**Introduction:**

Notes written while following Dr. Alannah Hallas's PHYS 474 UBC lecture notes. If any errors are found in the notes, feel free to email me at tobias.faehndrich@gmail.com. Overleaf formatting was copied from Rio W.

# Contents

# 1 Introduction

This lecture talked about the course structure, grading and basic questions about solid state physics and why it is important.

# 2 Heat Capacity Models I — Boltzmann and Einstein

Chapter 2 covers the Specific Heat of Solids

Recall:

- Heat capacity of material is how much energy (heat) you need to add to change the temp (by 1K).

$$C = \frac{d \langle E \rangle}{dT} \tag{2.1}$$

- Solids are incompressebile so $C_v \simeq C_p$

- "specific heat" and "heat capacity" are used interchangeably

- strictly we are speaking about molar heat capacity (per mol of material) with units of $[J/\text{mol} \cdot K]$

- 
$$1 \, \text{mol} = N_A = 6.022 \times 10^{23}$$

Why do we care?

- gives us info about thermally excited states and so we can look for phase transitions

- largest factor in specific heat is atomic vibrations

Heat capacity of an ideal monoatomic gas at constant volume (3-D)

- Equipartiion theorem: each quadratic degree of freedom in the energy contributes $\frac{1}{2}k_B T$ to $\langle E \rangle$

- Ideal Gas only has kinetic energy with x, y, and z components so we get

$$\langle E \rangle = \frac{3}{2}k_B T \tag{2.2}$$

per atom

$$\langle E \rangle = \frac{3}{2}RT \tag{2.3}$$

per mol

$$C = \frac{d \langle E \rangle}{dT} = \frac{3}{2}R \tag{2.4}$$

- Note that:

$$R = N_A \cdot k_B = 8.314 J/\text{mol} \, K$$

Experimental observations from 1820-1910

- Dulong-Petit Law:

$$C = 3k_B \tag{2.5}$$

per atom (or $C = 3R$ per mol)

- Boltzmann made classical statistical model that explained the Dulong-Petit result

  - It treated each atom as a **simple harmonic oscillator**
  - each of which were held in place in each direction by a spring vibrating t a frequency, $\omega$.

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{k\hat{x}^2}{2} \tag{2.6}$$

where $\omega = \sqrt{\frac{k}{m}}$ which you will show on HW1 that it gives $C = 3R$

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– But this still does not explain diamond or any solid significantly below room temperature

- Thermodynamics refresher

  – The probability of finding a system, S, that is in thermal equilibrium with a reservoir, R, at some temperature, T, in a given energy state, $E_i$,
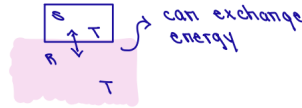


  is given by

  $$\mathbb{P}(E_i) \propto e^{-\beta E_i}$$

  where $\beta = \frac{1}{k_B T}$ with units of $\left[\frac{1}{\text{energy}}\right]$
  Note that the exponential term is the Boltzmann distribution

  – We can use the **partition function (Z)** to normalize our probabilities.
  i.e. so that we get $\sum_i \mathbb{P}(E_i) = 1$

  $$\mathbb{P}(E_i) = \frac{e^{-\beta E_i}}{e^{-\beta E_1} + e^{-\beta E_2} + \ldots} = \frac{e^{-\beta E_i}}{Z}$$

  where $Z = \sum_i e^{-\beta E_i}$

  – The **expecation value (or thermal average)** for a given quantity is the sum of the possible values weighted by their normalized probabilities.

  $$\langle x \rangle = \sum_i x_i \mathbb{P}(E_i) = \sum_i x_i \left(\frac{e^{-\beta E_i}}{Z}\right) = \frac{1}{Z} \sum_i x_i e^{-\beta E_i}$$

  where $Z = \sum_i e^{-\beta E_i}$

  – Taking the **derivative of the partition function with respect to** $\beta$ we uncover a useful trick.

  $$\frac{dZ}{d\beta} = \sum_i (-E_i) e^{-\beta E_i}$$

  Divide by $-Z$ and we get

  $$\frac{-1}{Z}\frac{dZ}{d\beta} = \frac{1}{Z}\sum E_i e^{-\beta E_i} = \langle E \rangle$$

  Thus we get the equation that relates the average internal energy to the partition function.

  $$\langle E \rangle = \frac{-1}{Z}\frac{dZ}{d\beta}$$

  which is useful because we want to calculate $C = \frac{d\langle E \rangle}{dT}$

  – **Bose-Einstein** and **Fermi-Dirac Statistics** to describe the energy distribution of quantum particles

    * BE: photons, cooperes pairs, $He^4$, atomic vibrations (phonons)

· The Bose occupation factor $n_B$ gives the number of bosonic particles occupying a given energy state at a given temperature.
As $T \to 0$, all particles occupy the ground state.
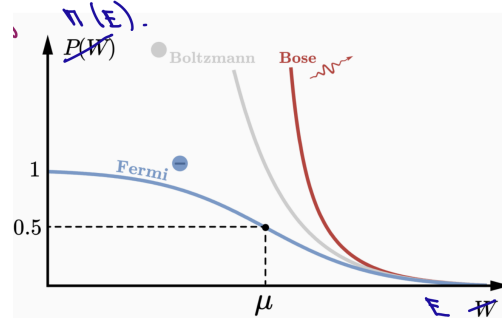


$$n_B = \frac{1}{e^{(E-\mu)\beta} - 1}$$

· where in the high T limit looks identical to Boltzmann distribution.
· as $T \to 0$, $\beta \to$ and only the lowest E state ($E \approx \mu$) is occupied
· and $\mu$ is the chemical potential (energy cost to add a particle to the system

* FD: electrons, other leptons, He$^3$
  · The Fermi factor $n_F$ gives the number of fermionic particles occupying a given energy state at a given temperature where each state can only be single occupied due to the Pauli exclusion principle.

$$n_F = \frac{1}{e^{(E-\mu)\beta} + 1}$$

· also looks identical to the Boltzmann distribution in the high T limit

# 3   Heat Capacity Models II — Einstein Revisited and Debye

**Einstein's model for specific heat**

- Einsten improved upon Boltzmann's model by treating each atom as a quantum mechanical simple harmonic oscillator, still being held in place in each spatial direction by a spring that vibrates at a frequency, $\omega$.

$$E_n = \hbar\omega\left(n + \frac{1}{2}\right)$$

  where $\omega$ is the frequency of the spring, and n is the quantum number.

- Note that in this model the atoms are still not connected to each other.

- You can follow the steps:

  1. Find $Z$
  2. $\langle E \rangle = \frac{-1}{Z}\frac{\mathrm{d}Z}{\mathrm{d}\beta}$,
  3. $C = \frac{\mathrm{d}\langle E \rangle}{\mathrm{d}T}$

  and then you get

$$C = 3R(\beta\hbar\omega)^2 \cdot \frac{e^{\beta\hbar\omega}}{(e^{\beta\hbar\omega} - 1)^2}$$

  Note that this expression depends on temperature!

- For HW1:

$$\sum_n x^n = \frac{1}{1-x} \quad \text{for } |x| < 1$$

  and

$$\sinh(x) = \frac{e^x - e^{-x}}{2}$$

- The **high T limit of Eistein's model** gives the expected **Dulong-Petit** value

$$\text{As} \quad T \to \infty, \beta \to 0$$

  You can taylor expand for the exponential term in the denominator

$$C \approx 3R(\beta\hbar\omega)^2 \cdot \frac{(1 + \beta\hbar\omega)^{\sim 0}}{(\beta\hbar\omega)^2}$$

$$\boxed{C = 3R} \quad \text{which is the Dulong Petit value!}$$

- The **low T limit** accounts for the observation that specific heat decreases with T
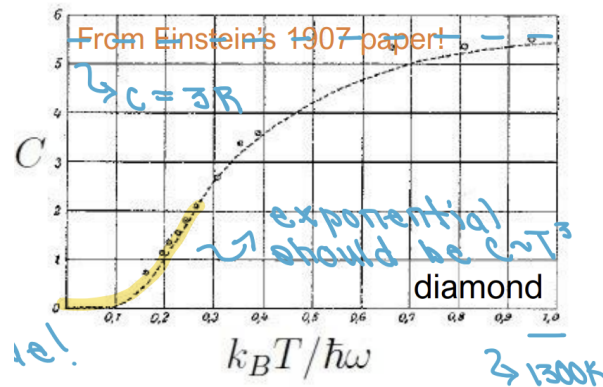
$$\text{As} \quad T \to 0, \beta \to \infty$$

$$C \approx 3R(\beta\hbar\omega)^2 \cdot \left(\frac{1}{e^{\beta\hbar\omega}}\right)$$

Correctly shows that

$$\text{As} \quad T \to 0, C \to 0$$

And also the discrepancy for diamond where C increased to 3R above room temp.

But incorrectly suggests an exponential decrease at low T. The data (Einstein's 1907 paper) showed that at low T, $C \sim T^3$.



- Einstein temperature is then defined as

$$T_E = \frac{\hbar\omega}{k_B}$$

where you can think of a materials hardness to be related to the stiffness of the spring holding it in place

$$T_E \propto \omega, \quad \text{and} \quad \omega = \sqrt{\frac{k}{m}}$$

so that the the mass of the atom also determines this temperature.

- You can calculate the typical frequency scale using a typical Einstein temperature using

$$f = \frac{\omega}{2\pi}$$

**Debye's model for specific heat**

- Debye took Einstein's calculation one step further by realizing that **the atomic vibrations in solids are sound waves** and therefore – not only should the energy levels be quantized – but the energy should vary as a function of the wave vector, k.

  - Einstein: $\omega = $ constant
  - Debye: $\omega(\vec{k}) = v|\vec{k}|$

- How should we think about the wavevector, k?

  e.g. 2D plane wave?

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$$\vec{k} = \frac{2\pi}{\lambda}\hat{k}$$
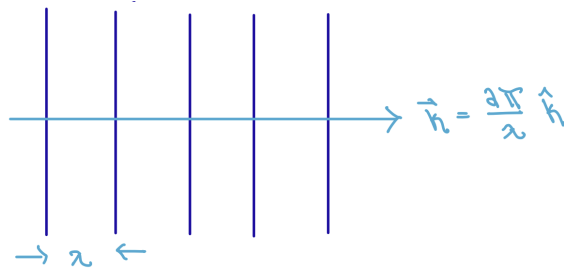
k-space is useful because solids are periodic

other names:

- momentum space
- reciprocal space
- Q space

Normal space is called " real space "

**Periodic (Born-von Karman) boundary conditions** (equivalet to particle in a box, but easier)

- Rather than treating our solids as having fixed end points, it is very convenient to apply **periodic boundary conditions**.

- In 1D this means taking a very long chain and attaching the ends together.

- Surfaces account for only a tiny fraction of a material so this is a reasonable thing to do.
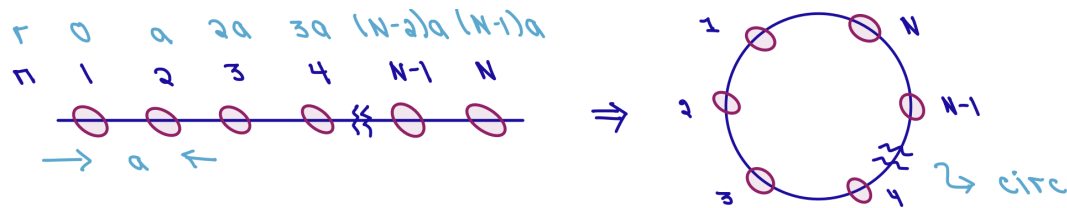


$$L = N \cdot a$$

- This imposes a condition on the possible k-values: the values of k are quantized!

- A wave $e^{ikr}$ must have the same value at r and $r + L$:

$$e^{ikr} = e^{ik(r+L)} \Rightarrow e^{ikL} = 1 \Rightarrow k \cdot L = 2\pi n \quad (n = \text{integer})$$

$$\boxed{k = \frac{2\pi}{L}n}$$

k is quantized! and $\Delta n = 1 \Rightarrow \boxed{\delta k = \frac{2\pi}{L}}$ so that $L \gg 1$, then $\delta k \ll 1$.

- In 3D ($v = L^3$) we can use the same trick excep the solid gets folded into a hypertorus.

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- allowed k states $\quad \vec{k} = \frac{2\pi}{L}(n_x, n_y, n_z)$

- Volume of a k-point ($\Delta n_i = 1: \quad \delta k = \left(\frac{2\pi}{L}\right)^3$

- Since the number of allowed wave vectors is discrete, we can count them:

$$\text{\#k-points} = \sum_k = \frac{\text{volume of k space}}{\text{volume of k point}} = \frac{\int d\vec{k}}{\left(\frac{2\pi}{L}\right)^3}$$

- We can convert the sum over all k to a 1D integral (assume spherical symmetry).

$$\int_{-\infty}^{\infty} d\mathbf{k} \rightarrow \int_0^{\infty} d\varphi \int_0^{\pi} d\theta \sin(\theta) \cdot \int_0^{\infty} k^2 \, dk$$

For the 3D. Can check 2D and 1D too.

- Now pulling the pieces together for Debye's model, we can calculate the specific heat by starting with an expression analogous to Einstein's except where $\omega$ depends on $\mathbf{k}$.

  - Einstein:

$$\langle E \rangle = 3\hbar\omega \left[ n_B(\beta\hbar\omega) + \frac{1}{2} \right]$$

  (from $\langle E \rangle = \frac{-1}{Z}\frac{dZ}{d\beta}$)

  - Debye:

$$\langle E \rangle = 3\sum_{\mathbf{k}} \hbar\omega(\mathbf{k}) \left[ n_B(\beta\hbar\omega(\mathbf{k})) + \frac{1}{2} \right]$$

  (where $\omega = v|\vec{k}|$)

- We can use the relationship above to then convert our sum to an integral –¿ Then, it is preferable to evaluate this integral with respect to $\omega$ instead of $k$.

  1. Convert $\sum_{\vec{k}}$ to $\int d\vec{k}$
  2. Convert 3D integral to 1D
  3. 3 Change of variable , $k = \frac{\omega}{v}$, $dk = \frac{1}{v} d\omega$
  4. Result:

$$\langle E \rangle = \int_0^{\infty} d\omega \cdot \left[ L^3 \cdot \frac{12\pi\omega^2}{(2\pi)^3 v^3} \right] \hbar\omega \left( n_B(\beta\hbar\omega) + \frac{1}{2} \right)$$

Note the velocity term!

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