Midterm, From Atoms to Solids II, Friday, May 29, 2026

Total number of points: 90, Grade=1+1/10*points Model answers on p. 3-5

1: Einstein and Debye model (4+4+4=12 pt)

(a) In the Einstein model, lattice vibrations are quantised.
Explain qualitatively how this quantization modifies the heat capacity at low temperature.

(b) Sketch qualitatively the heat capacity as a function of temperature predicted by:

- classical theory
- Einstein model

(c) State one improvement introduced by the Debye model compared with the Einstein model.

2: Drude and Sommerfeld model (5+5+5+8=23 pt)

(a) Derive the Drude expression:

$$\sigma = \frac{ne^2\tau}{m}$$

(b) The electronic heat capacity of metals is experimentally found to be much smaller than predicted by the classical Drude model. Using the Sommerfeld model, explain qualitatively:

- why only a fraction of electrons contribute to the heat capacity,
- why the heat capacity is approximately proportional to temperature at low T.

(c) Show that the dispersion of a 1D free electron gas (with electrons described as plane waves) is $E(k) = \frac{\hbar^2|k|^2}{2m}$.

(d) Derive an expression for the Fermi energy in terms of electron density $n = N/V$:

$$E_F = \frac{\hbar^2(3\pi^2 n)^{\frac{2}{3}}}{2m}$$

Hint: Express the electron number N by an integral over k-space using the appropriate k-space volume occupied by a single state. Evaluate the integral at $T = 0$.

3: Vibrations in the monoatomic linear chain (4+5+5+5=19 pt)

(a) Give the expression for the dispersion relation of the 1D monoatomic linear chain and one for its long-wavelength limit.

A one-dimensional monoatomic linear chain consists of identical atoms of mass $m = 1.0 \times 10^{-26}$ kg, separated by a lattice constant $a = 0.25$ nm. The atoms are connected by identical springs with a force constant $\kappa = 10$ N/m.

(b) Calculate the maximum angular frequency in the Brillouin zone for this 1D monoatomic linear chain.

(c) Calculate the group velocity around $k = 0$ (that is, evaluate for the low k limit) and give its physical significance.

(d) Describe qualitatively, how the dispersion relation for vibrations changes when going to a diatomic or a triatomic chain, respectively.

4: 1D tight-binding chain (4+5+5+4=18pt)

Consider a one-dimensional chain of identical atoms with one s-orbital per atom. The electrons can hop between nearest-neighbor sites only, with a hopping (transfer) integral $t > 0$.The lattice spacing is a and the chain is infinite.

(a) Write down the expression for the energy dispersion relation $E(k)$ in the tight-binding approximation. Sketch the band structure for the first Brillouin zone.
(b) Determine the bandwidth and the location of the maximum and minimum energy in k-space.
(c) Show that the effective mass at the bottom of the band is given by $m^* = \frac{\hbar^2}{2ta^2}$.
(d) Briefly explain the concept of the effective mass qualitatively.

5: Crystal structure and reciprocal lattice (5+6+7=18 pt)

Consider a 3D body-centered cubic (bCC) crystal with lattice constant $a = 0.32$ nm.

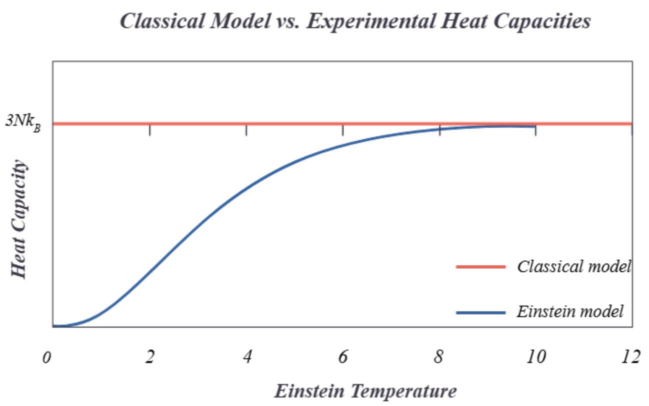
(a) How many atoms are contained in the conventional cubic unit cell? Calculate the volume of the conventional unit cell.
(b) Determine the magnitude of the shortest non-zero reciprocal lattice vector corresponding to the (110) family of planes and what is the distance between adjacent (110) planes?
(c) The (010) diffraction peak is absent in a BCC crystal. Show mathematically why this peak has zero intensity using the concept of the structure factor.

Solutions:

1: Einstein and Debey model (12 pt)

(a) In the Einstein model, atoms vibrate as quantum harmonic oscillators with discrete energy level. At low temperature, the thermal energy becomes too small to excite many vibrational modes. As a result, fewer oscillators contribute to the internal energy, causing the heat capacity to decrease. This differs from classical theory, where all oscillators contribute equally at all temperatures and the heat capacity remains constant.

(b)



(c)

The Debye model improves on the Einstein model by allowing a continuous spectrum of phonon frequencies rather than assuming all atoms oscillate with the same frequency. As a result, the Debye model correctly predicts the low-temperature behaviour: $c_V \propto T^3$which agrees with experiment.

2. Sommerfeld Model (28 pt)

(a) Drude derivation, Simon, page 20

(b)

- only electrons near the Fermi surface contribute to specific heat (because $kT \ll E_F$)
- assuming the density of states approximately constant at E_F, the number of relevant electrons is proportional to $g(E_F)k_BT$, so it increases linearly with T and so does the heat capacity.

(c)

We are dealing with de Broglie waves, i.e.:
$E = \frac{p^2}{2m}$ and $p = \hbar k$, from this $E(k) = \frac{\hbar^2|k|^2}{2m}$ follows. Alternatively, you can obtain it from the Schrödinger equation for a free electron described as a plane wave.

(d)

$$N = 2\sum_{\vec{k}} n_F\left(\beta\left(\epsilon(\vec{k}) - \mu\right)\right) = 2\frac{L^3}{(2\pi)^3}\int n_F\left(\beta\left(\epsilon(\vec{k}) - \mu\right)\right) d\vec{k}$$

Integrate up to k_F, convert to particle density, solve for k_F and plug in the dispersion relation from (a).

3. Vibrations in the monoatomic linear chain (20 pt)

(a) $\omega = 2\sqrt{\left(\frac{\kappa}{m}\right)}\left|sin\left(\frac{ka}{2}\right)\right|$

Long wavelength limit: $\omega = 2\sqrt{\left(\frac{\kappa}{m}\right)}\left|\frac{ka}{2}\right| = a\sqrt{\left(\frac{\kappa}{m}\right)}\,|k|$

(b) Maximum occurs at BZ edge, i.e. $k = \pm\frac{\pi}{a}$, i.e. $\omega = 2\sqrt{\left(\frac{\kappa}{m}\right)} = 6.32 \times 10^{13}\,rad/s$

(c) $v_{group} = \frac{d\omega(k)}{dk} = a\sqrt{\left(\frac{\kappa}{m}\right)}$ in the low k limit.

$v_{group} = 7.91 \times 10^3\,m/s$

At low k ,the group velocity gives the speed of sound.

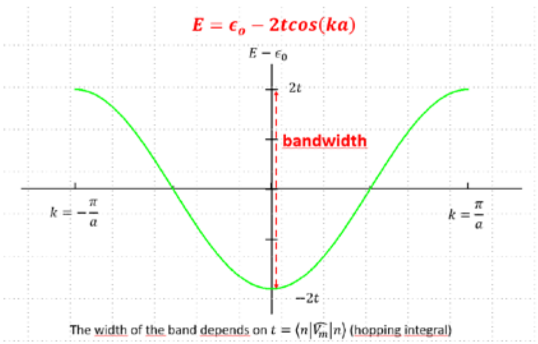
(d) Diatomic chain: An optical phonon branch opens up

Triatomic chain: Two optical phonon branches

Both branches have finite energy at k=0, but flat dispersion (standing waves)

4. Tight binding chain (20 pt)

(a) $E = \epsilon_o - 2tcos(ka)$



(b) $\Delta E = 4t$

E_min = ε_0 - 2t at k = 0

E_max = ε_0 + 2t at k = +- π/a

(c) $E = \epsilon_o - 2t\cos(ka) \approx const + ta^2k^2$

$$E_{free} = \frac{\hbar^2 k^2}{2m}$$

$$\frac{\hbar^2 k^2}{2m^*} = ta^2k^2$$

(d) The effective mass describes how an electron in a crystal responds to forces as if it were a free particle with a different mass due to interactions with the periodic lattice potential.

5. Crystal structure and reciprocal lattice (20 pt)

(a) In a BCC lattice, 8 corners contribute 1/8 atom, each. 1 atom in the center needs to be added. Total is 2. The volume of this cubic cell is $a^3 = 0.3^3$ nm^{3}0.033nm^3.

(b) $|\vec{G}| = \frac{2\pi}{a}\sqrt{h^2+k^2+l^2} = \frac{2\pi}{a}\sqrt{1^2+1^2+0^2} = \frac{2\pi}{a}\sqrt{03} = 27.77$ nm^{-1}

$d = \frac{2\pi}{|\vec{G}|} = 0.226$ nm

(c) The BCC lattice contains two atoms in the basis: (0,0,0) and (1/2,1/2,1/2)

The structure factor is:

$S_{(hkl)} = f_{Cs} + f_{Cs}e^{i2\pi(h,k,l)\left(\frac{1}{2},\frac{1}{2},\frac{1}{2}\right)} = f_{Cs} + f_{Cs}e^{i\pi(h+k+l)} = f_{Cs}\left(1 + (-1)^{(h+k+l)}\right)$

(100) : h + k + l = 1 (odd)

Destructive interference, no intensity