Condensed Matter Physics Final Exam December 2, 2019

Total: 100 Marks

- 1. Consider a thin film of solid material (one atom thick) arranged in a square lattice with area $A = L \times L$, deposited on an inert substrate. The N atoms may vibrate parallel to the substrate, but not perpendicular to it. The speed of sound in the solid is c_s .
 - (a) Find the vibration frequency ν as a function of L and c_s .
 - (b) Show that the density of vibration modes as a function of vibration frequency ν is $D(\nu) = 4\pi A\nu/c_s^2$.
 - (c) Verify that the maximum vibration frequency $\nu_{\rm max}$ is

$$\nu_{\rm max} = \left(\frac{c_s^2 N}{\pi A}\right)^{1/2} {\rm Hz}.$$
 (1)

- (d) What is the temperature of the system at which all the modes are excitable (Debye temperature)? What does the Debye temperature tell us about the heat capacity of the material?
- (e) Calculate the average energy $\langle E \rangle$ and the heat capacity at constant area C_A in the limit of
 - i. high temperature $k_B T \gg h\nu_{\text{max}}$. Note: for small $x, e^x = 1 + x$.
 - ii. low temperature $k_B T \ll h \nu_{\text{max}}$.

Note:
$$\int_0^\infty \frac{x^2}{e^x - 1} dx = 2.404.$$
 (2)

(f) (Briefly) describe an experimental setup to determine the heat capacity of such a material.

(30 Marks) (Note: for 20 Marks you can solve the entire problem considering only perpendicular vibrations).

- 2. In certain materials, particularly at higher temperature, positive ions can move throughout the sample in response to applied electric fields, resulting in what is known as ionic conduction. Since this conduction is typically poor, it is mainly observable in materials where there are no free electrons that would transport current. However, occasionally it can occur that a material has both electrical conduction and ionic conduction of roughly the same magnitude such materials are known as mixed ion-electron conductors. Suppose free electrons have density n_e and scattering time τ_e (and have the usual electron mass m_e and charge e). Suppose that the free ions have density n_i , scattering time τ_i , mass m_i and charge +e. Using Drude theory,
 - (a) Calculate the electrical resistivity.
 - (b) Calculate the thermal conductivity.

(20 Marks)

3. Consider a one-dimensional periodic potential V(x) as shown in the figure below. An electron moves in this one-dimensional crystal of length L. The regions denoted II correspond to the positively charged ions of the crystal lattice. The regions denoted I represent the empty spaces between the ions. The lattice parameter is a = d + s.



- (a) Set up the single-electron Schrödinger equation for this system (in the two regions).
- (b) What are the eigenfunctions of this Hamiltonian (Hint: You can guess these using Bloch's theorem, don't forget the reflected wave!). Determine the relevant constants using the boundary conditions and the normalization.
- (c) What are the conditions for a solution to exist? Sketch the energy levels for this system (are there band gaps?).

(25 Marks)

4. A specimen in the form of a cube of side L has a primitive cubic lattice whose mutually orthogonal fundamental translation vectors (primitive lattice vectors) have length a. Show that the number of different allowed k-states within the first Brillouin zone equals the number of primitive unit cells forming the specimen. (You may assume periodic boundary conditions. What about for hard-wall boundary conditions?)

(10 Marks)

5. In the tight binding model we assume that there is a single orbital on atom n which we call $|n\rangle$. Consider these orbitals to be the (1d analogues) of the ground state wavefunction of the hydrogen atom given by

$$|n\rangle = \frac{1}{\sqrt{a_0}} e^{-|x-x_n|/a_0},$$
(3)

where x_n represents the mean position of the n^{th} orbital.

- (a) Compute the overlap integral s for electrons on adjacent sites. For what lattice spacing a is the assumption of orthogonality of adjacent orbitals valid? (Use $a_0 = 5.292 \times 10^{-11}$ m).
- (b) Sketch the effect of systematically increasing the lattice spacing on the dispersion relations (i.e. taking the $s \rightarrow 0$ limit, qualitatively will do).