THE UNIVERSITY OF NEW SOUTH WALES

SCHOOL OF PHYSICS

FINAL EXAMINATION

June 2014

PHYS3080 Solid State Physics

PHYS3021 Statistical and Solid State Physics

1. Time Allowed: 2 hour
2. Total number of questions: 5
3. Marks available for each question are shown in the examination paper. The total number of marks is 60.
4. Attempt ALL questions!
5. Candidates must supply their own, university approved, calculators.
6. Answers must be written in ink. Except where they are expressly required, pencils may only be used for drawing, sketching or graphical work.
7. The exam paper may be retained by the candidate.

Data and Formula Sheet†

NB: This is a generic PHYS3080 data/formula sheet and contains some additional information you may not necessarily need for this exam.

$$\vec{a}^* = 2\pi \frac{(\vec{b} \times \vec{c})}{\vec{a} \cdot (\vec{b} \times \vec{c})} \quad \text{and anticyclical permutations of the numerator}$$

$$e^x = 1 + x + \frac{x^2}{2} \cdots, \qquad \int_0^{\Theta_D/T} \frac{x^4 e^x}{(e^x - 1)^2} dx \approx \int_0^{\infty} \frac{x^4 e^x}{(e^x - 1)^2} dx \approx \frac{4\pi^4}{15}$$

$$\dot{Q} = \frac{dQ}{dT} = \kappa A \frac{dT}{dx}, \qquad c_V = \tfrac{1}{2} k_B T \text{mole}^{-1} \text{ per degree of freedom}$$

$$\kappa = \tfrac{1}{3} \nu l c, \qquad R = k_B / N_A, \qquad E_{Th.} = k_B T$$

$$\epsilon_{CB}(k) = E_{\text{Gap}} + \frac{\hbar^2 k^2}{2 m_e^*}, \qquad \epsilon_{VB}(k) = -\frac{\hbar^2 k^2}{2 m_h^*}$$

$$v_{\text{Gr}} = \tfrac{1}{\hbar} \text{grad}_k \epsilon(k), \qquad \frac{1}{m^*} = \frac{1}{\hbar^2} \frac{\partial^2 \epsilon(k)}{\partial k_x^2}$$

$$E_n = -\frac{m_e^* e^4}{8 h^2 n^2 \varepsilon_0^2}, \qquad a = a_0 \epsilon_r \left(\frac{m_e}{m_e^*} \right), \qquad a_0 = 0.53 \text{Å}$$

$$n_n p_n = n_i^2 = n_p p_p, \qquad n_i = p_i = \sqrt{N_{CB} \cdot N_{VB}}\; exp(-E_{\text{Gap}}/2 k_B T),$$

$$n_D \approx N_{CB}\; exp(-E_D / k_B T) \text{ for } k_B T \ll E_D,$$

$$p_A \approx N_{VB}\; exp(-E_A / k_B T) \text{ for } k_B T \ll E_A$$

$$\vec{F} = q(\vec{v} \times \vec{B}), \qquad I = NAve, \qquad v = -\frac{e\tau}{m_e} E$$

$$J = \sigma E, \qquad \sigma = ne\mu = \frac{ne^2 \tau}{m_e}, \qquad \mu = \frac{v_d}{E}, \qquad R_H = -\frac{1}{ne}$$

$$j = j_0 \sin \left[\frac{2e}{\hbar} \left(V_0 t + \frac{V}{\omega} \sin(\omega t) \right) \right], \qquad V_0 = \frac{n\hbar\omega}{2e} = \frac{nh\nu}{2e}$$

$$n_{\text{phonon}} \sim \exp(-\Theta_D / T), \qquad \lambda_{\text{phonon}} \sim \exp(+\Theta_D / T)$$

$$k_F = \left(\frac{3\pi^2 N}{V} \right)^{1/3}, \qquad \xi_0 = \frac{\hbar v_F}{\pi \Delta_0}$$

$$\sin(2\theta) = 2 \sin(\theta) \cos(\theta)$$

$$e = 1.6 \cdot 10^{-19}\ C, \qquad \varepsilon_0 = 8.854 \cdot 10^{-12}\ Fm^{-1}, \qquad N_A = 6.023 \cdot 10^{23}\ g/\text{mole}$$

$$h = 6.63 \cdot 10^{-34}\ Js, \qquad \hbar = 1.05 \cdot 10^{-34}\ Js, \qquad \lambda_{\text{visible}} \sim 400 - 700\ nm$$

$$k_B = 1.380658 \cdot 10^{-23} J/K, \qquad m_e = 511\ keV = 9.109 \cdot 10^{-31} kg$$

Question 1 (10 marks)

Neutron Diffraction

(a) Neutrons emitted from a research reactor posses a broad energy spectrum. How can you obtain monochromatic neutrons with precisely one wavelength?

(b) Name three different diffraction techniques.

(c) Give a brief description of one diffraction technique, including a schematic figure.

(d) In order to determine the crystal structure of a solid, neutrons with a wavelength of 1.6 Å can be used. The distance between the atoms in a cubic crystal is for example $d = 3.2$ Å. Calculate the diffraction angles of the first, second, and third order Bragg refection. A flat plate neutron detector is placed 30 cm from the crystal. At which distance from each other do the three Bragg reflections appear on the detector?

Question 2 (10 marks)

Explain the following, each in a few words

(a) Give the expression for the reciprocal lattice vectors and explain the relation between the vectors in real space and reciprocal space by multiplying them.

(b) Sketch all branches of the phonon dispersion relation of a bi-atomic three dimensional lattice and label them.

(c) Explain the terms metal, insulator, semiconductor, and semi-metal in terms of band-filling. Give a sketch of each of the different band structures.

(d) Explain why electrons in a completely filled band, in particular in case of an insulator, do not contribute to the electronic conductivity.

(e) Give one example of a solid state particle which follows the Fermi-Dirac and one which follows the Bose-Einstein statistics.

Question 3 (15 marks)

(i) Density of States of a free Electron

Calculate the density of states ($D(\epsilon)$) of free electrons using the known energy dispersion ($\epsilon(\vec{k}) = \frac{\hbar^2 k^2}{2m_e}$) for the 1-, 2-, and 3-dimensional case.

simplify if necessary

(ii) Dispersion Relation

Consider a crystal where the energy dispersion relation is given by:

$$\epsilon(k_x) \;=\; \epsilon_1 \pm (\epsilon_2 - \epsilon_1)\sin^2(ak_x/2) \;,$$

where ϵ_1 and ϵ_2 are constants.

(a) Sketch and label the energy dispersion relation of both branches in the Brillouin zone.

(b) Assume one electron in the band and calculate the electron velocity, i.e. the group velocity. $d\epsilon/dk$

(c) calculate the effective mass of the electron ($\frac{1}{m^*} = \frac{1}{\hbar^2}\frac{\partial^2 \epsilon}{\partial k_x^2}$).

(d) Sketch the behaviour of electron velocity and the effective mass throughout the Brillouin zone.

(e) Where are the electrons and holes located in the Brillouin zone?

Question 4 (15 marks)

Specific Heat of a Insulator

(a) Give the equation of the Bose-Einstein distribution function and explain all symbols in this expression.

(b) What is the Debye model and what is the Einstein model. Explain both models and sketch the Density of States as a function of energy. Which phonons are represented by the Debye model and which by the Einstein model?

(c) Calculate the specific heat in the case of the Debye model.

$$U_{\text{osz.}}(T) \;=\; \sum_{\nu} D_{DE}(\omega)\,\hbar\omega(f_{\text{BE}}(E_\nu, T) + 1/2)$$

$$c_V(T) \;=\; \left(\frac{d\,U_{\text{osz.}}(T)}{dT}\right)_T$$

$$\text{where :} \qquad D_{DE}(\omega) = \frac{9N}{\omega_{DE}^3}\cdot\omega^2 \qquad \text{for } \omega \le \omega_{DE}$$

(d) Use the approximation for the solution of the integral given on the 'Data and Formula Sheet' to derive that the specific heat converges with T^3 towards $T = 0K$.

(e) Plot the specific heat of an insulator in the entire temperature range.

Question 5 (10 marks)

Metallic Conductivity

The Fermi-Dirac distribution function gives the occupation probability of the states of the electrons in a free electron metal:

$$f(\epsilon, T) = \frac{1}{1 + e^{\frac{\epsilon - \epsilon_F}{k_B T}}}$$

(a) Define all symbols in this expression.

(b) The total number of occupied electron states, $N(\epsilon)$, in the energy range $\epsilon \rightarrow \epsilon + d\epsilon$ is given by the product of the occupation probability $f(\epsilon, T)$ with the function of the density of states $g(\epsilon)$.
Sketch the three quantities $N(\epsilon)$, $f(\epsilon)$, and $g(\epsilon)$ for a simple three-dimensional free electron gas of a metal. Indicate the situation for $T = 0K$ and $T_F \gg T > 0K$, where T_F is the Fermi temperature.

(c) Give a concise explanation of the reason that the observed electronic (i.e. the conduction electrons) contribution to the specific heat capacity of a metal is only a small fraction of that expected classically. Refer to the sketch of question 5(b) to explain your answer.

(d) What is the temperature dependence of the electronic contribution to the specific heat. Do not derive this expression, just give a sketch of the function.