

THE UNIVERSITY OF NEW SOUTH WALES

SCHOOL OF PHYSICS

FINAL EXAMINATION

PHYS 4103 – 2016

Solid State Physics

1. Time Allowed: 3 hours
2. Total number of questions: 9
3. Marks available for each question are shown in the examination paper.
The total number of marks is 100.
4. Attempt ALL questions!
5. Question 1-4, 5, and 6-10 must be answered in a separate book.
6. Candidates may bring their own calculators (calculators without alphabetic keyboards).
7. Answers must be written in ink. Except where they are expressly required, pencils may only be used for drawing, sketching or graphical work. Do not use red ink.
8. The paper may be retained by the candidate.

Question 1 (12 marks): Explain briefly

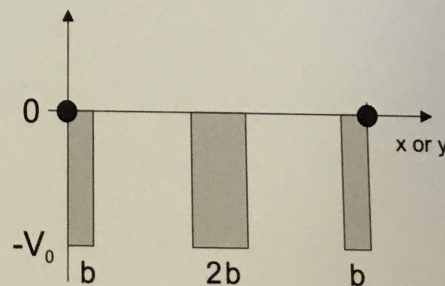
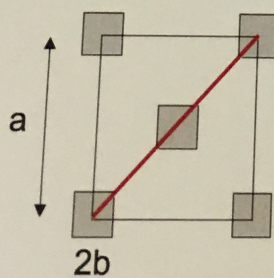
- (a) Construction of the Hamilton operator of a solid: give and explain the various terms which contribute to the Hamilton operator of a solid.
- (b) What is the main problem to solve the Schrödinger equation of a solid directly? Various approximations are required to solve the Schrödinger equation of the electronic system of a solid numerically. Explain two approximations in detail.
- (c) The electronic band-structure of a solid can be calculated using the „Tight Binding Limit“. Explain this technique briefly in a few words.
- (d) Give a brief sketch of the electronic band structure of a metal, semi-metal, insulator, direct semiconductor and indirect semiconductor.
- (e) Explain the experimental setup of a photoluminescence setup. Give a brief sketch and label the various components.
- (f) Explain the photoluminescence technique in a few words and explain the excitation and emission process. Use a sketch of the Valence band maximum and Conduction band minimum for your explanation. What is the difference between a photoluminescence experiment on a direct semiconductor and that on an indirect semiconductor?

Question 2 (14 marks):

Weak Binding Limit:

A direct way to calculate the electronic band structure of a crystal is the „weak binding limit“, which is starting from the dispersion of a free electron:

- (a) Explain the technique of the „weak binding limit“ by using a sketch of the first Brillouin zone of a solid.
- (b) Calculate the two-dimensional band structure in the „weak binding limit“. Consider a two-dimensional square lattice with the lattice constant a with one electron per lattice site. The electrons interact with the nuclei through a weak two-dimensional box-potential as follows:



$$V(x, y) = -V_0, \quad \text{with } |x|, |y| < b$$

$$V(x, y) = 0, \quad \text{otherwise}$$

Calculate the electronic band structure in the weak binding limit along the $\vec{k} = (\pi/a, \pi/a)$ direction of the Brillouin zone. Use the following relations for the diagonal and off-diagonal matrix elements:

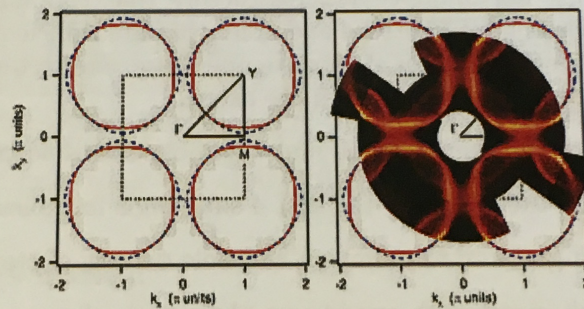
$$\langle \varphi_0(k) | H_1 | \varphi_0(k) \rangle = \frac{1}{A} \int_{\text{crystal}} e^{ikr} V(r) e^{-ikr} d\vec{r} = \frac{1}{a^2} \int_{\text{unit cell}} V(r) d\vec{r} = \text{const.}$$

$$\langle \varphi_0(\vec{k}) | H_1 | \varphi_0(-\vec{k}) \rangle = \frac{1}{a^2} \int_{\text{unit cell}} e^{2i\vec{k}\vec{r}} V(\vec{r}) d\vec{r}$$

Question 3 (8 marks):

Angular Resolved Photo-Emission Spectroscopy:

- (a) Give a brief sketch of the experimental setup of the ARPES technique (Angular Resolved Photo-Emission Spectroscopy) and label the various components.
- (b) How can the electronic band structure be measured using the technique ARPES? Give a sketch of the corresponding band structure and denote the observed transitions.
- (c) The figure below shows the theoretical model and the ARPES data of the Fermi surface of a 2-dimensional layered material (the superconductor $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_8$). Explain the deviations of the Fermi surface at the zone boundary from a perfect circle in terms of the 'weak binding limit' approximation.



Question 4 (16 marks): Optical Absorption

The optical absorption coefficient is given by:

$$\begin{aligned} \alpha(\omega) &= \frac{2\pi e^2 \omega}{\epsilon_0 c_0 n} \int_{\text{BZ}} \frac{d\vec{k}}{4\pi^3} |M_{CV}|^2 \delta(E_c(\vec{k}) - E_v(\vec{k}) - \hbar\omega) \\ &= \frac{2\pi e^2 \omega}{\epsilon_0 c_0 n} |M_{CV}|^2 J_{CV}(\hbar\omega) \end{aligned}$$

where c_0 is the speed of light and n is the index of refraction of the material.
 J_{CV} is the joint density of states.

(a) Briefly sketch the experimental setup of an optical absorption experiment.

(b) Explain the terms „Van-Hove Singularity“ and „Joint Density of States“ briefly. Where do the Van Hove singularities appear in the electronic band-structure? Why do Van Hove singularities always appear at the zone centre and zone boundary of the Brillouin zone?

(c) Calculate the joint density of states for direct interband transitions for both, a three-dimensional band minimum and a two-dimensional band minimum in the electronic band structure.

Note:

$$\int g(x) \delta(f(x)) dx = \sum_{x_0} \left| \frac{df}{dx} \right|_{x=x_0}^{-1} g(x_0) \quad (1)$$

Question 5 (15 marks):

This question focusses on charge carriers in a semiconductor structure at room temperature. You can find the band offsets and masses listed at the end of the exam.

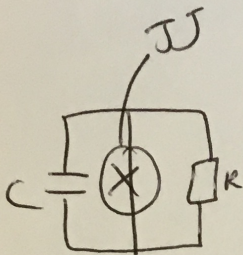
1. Construct an un-doped heterostructure that contains a 20 nm wide quantum well for electrons and holes that are sufficiently deep to bind the first few sub-bands at room temperature. Sketch the band structure and indicate the materials in the sketch.
2. Calculate the energy of the first 4 sub-bands for electrons in the well.
3. Calculate the energy of the first 4 sub-bands for holes in the well.
4. Sketch a graph of the electron and hole density of states of this well.
5. At which wavelength would you observe the first exciton absorption for this well?

Question 6 (6 marks):

In the lectures we have intensively discussed the derivation of the first Josephson equation, $J = J_C \sin(\phi)$. Can you anticipate what will happen to J in this formula in the case the junction has a very thick oxide layer (i.e. $a \gg 1$) instead of a very thin one like in the lectures. Can you also anticipate what will happen to J in this formula in the case $T \gg T_{critical}$, i.e. the temperature of the measurements is much higher than the critical temperature of the superconducting leads?

Question 7 (10 marks):

During the lectures we have introduced a model called the *Resistively and Capacitively shunted Junction (RCSJ) model*, which allows the description, in a simple and direct way, of the dynamical evolution of a real Josephson Junction (JJ). Without repeating the calculations leading to the introduction of this model, can you:



1. Schematically draw the basic electrical circuit elements that are assumed to be present in this model?
2. Briefly (2-3 sentences) explain the main advantages of this model?
3. Discuss which „order parameter“ can be used to describe the overall properties of a Josephson Junction according to this model?

junction of quasi particles

→ real JJ. shunting capacitor resistor

ϕ → phase diff.

According to this RCSJ model, which system can be used as a „classical“ equivalent to the „quantum“ Josephson Junction one? Once more, you don't need to write all the calculations but just to briefly outline the most important conclusions and the most important properties that are a consequence of the introduction of this model. Lastly, in this model we have introduced the quality factor, Q , and we have discussed the general effect of being in one of these two limits a) $Q \ll 1$ and b) $Q \gg 1$. Can you briefly discuss what is the main difference in the I-V behaviour of the junction that can be anticipated from these two a) and b) limits.

viscous fluid

Question 8 (9 marks):

Can you estimate, via Hund's rules as it has been done in the lectures, the values of S_{Cr} , L_{Cr} and J_{Cr} for Cr^{2+} knowing that the last 3d shell (hint: $n=3$) of this atom contains 4 electrons. Once you know the value of the J and by following the approach of the lectures, it is possible to anticipate that the magnetic properties of a particular material made of these Cr^{2+} atoms will be mostly dominated by only one kind of magnetism (between the ones that we have studied in the lectures). As a consequence of this:

1. Can you anticipate which kind of magnetism this material will have?
2. Can you, again by simply using the approach of the lectures, anticipate the kind of temperature dependence that the magnetic susceptibility ($\chi_m = \frac{M}{H}$) of this material is expected to have?

diatomic

T independent const.

Question 9 (5 marks):

1. Which one of the following formulas (a), (b), (c) and (d) is correctly representing the Brillouin function, i.e.: the function that can be used to describe, by means of a simple *quantum* model, the magnetisation of a paramagnetic/ferromagnetic systems under the influence of an external magnetic field H ?

(a) $\frac{2J+2}{2J} \operatorname{ctgh}\left(\frac{2J+2}{2J}y\right) - \frac{1}{2J} \operatorname{ctgh}\left(\frac{1}{2J}y\right)$

(b) $\frac{2J+1}{2J} \operatorname{tgh}\left(\frac{2J+1}{2J}y\right) - \frac{1}{2J} \operatorname{tgh}\left(\frac{1}{2J}y\right)$

(c) $\frac{2J+1}{2J} \operatorname{ctgh}\left(\frac{2J+1}{2J}y\right) - \frac{1}{2J} \operatorname{ctgh}\left(\frac{1}{2J}y\right)$

(d) $\frac{2J}{2J} \operatorname{sinh}\left(\frac{1}{2J}y\right) - \frac{1}{2J+1} \operatorname{sinh}\left(\frac{1}{2J}y\right)$

2. As it has been shown in the lectures, in the limit $J \sim \infty$, $B_J(y)$ is converging to the Langevin function, $L(y) = \operatorname{ctgh}(y) - \frac{1}{y}$, used to describe the magnetisation of a paramagnetic/ferromagnetic systems in the classical case. Can you briefly describe (by using not more than a few sentences) for which range of temperatures do you expect this „classical“ representation to be more accurate or alternatively for which range of temperatures this „classical“ representation is expected to be less accurate?

low \rightarrow Brillouin
high \rightarrow Langevin.

Question 10 (5 marks):

For an hypothetical magnetic material, in which the electronic configuration of the last shells of atoms leads to a positive value for the exchange integral, i.e. $J_{\text{Exchange}} \geq 0$, we can imagine to be in the hypothetical case (not possible in real systems) of having $J_{\text{Exchange}} \propto 1/(\text{distance})$ with a long range of action and the dipole-dipole forces having a short range of action (i.e.: $\propto \exp[-\text{distance}]$). Without the need of calculations, but just by using the intuitive approach discussed in the lectures, can you give a rough estimation of how many Weiss domains this hypothetical material would have?

0 or 1

The following may be needed:

- $T_{critical}$ is the critical current of material above which this material is not superconducting anymore.
- $k_B = 8.617 \cdot 10^{-5} \text{ eV/K}$
- $\mu_B = 9.27400968 \cdot 10^{-24} \text{ A m}^2$
- $\mu_0 = 1.256637 \cdot 10^{-6} \text{ Wb/(Am)}$
- $\Phi_0 = 2.06783376 \cdot 10^{-15} \text{ Wb}$
- $\epsilon_0 = 8.85 \cdot 10^{-12} \text{ F/m}$
- $h = 6.62 \cdot 10^{-34} \text{ J s}$
- $m_{electron} = 9.11 \cdot 10^{-31} \text{ kg}$
- $m_{e,AlAs}^* = 0.124$
- $m_{hh,AlAs}^* = 0.5$
- $m_{lh,AlAs}^* = 0.26$
- $m_{e,GaAs}^* = 0.067$
- $m_{hh,GaAs}^* = 0.51$
- $m_{lh,GaAs}^* = 0.082$

$$E_F = \frac{[k_B T] [k_B T] [k_B T]}{[k_B T] [k_B T] [k_B T]} = \frac{e^2 m_e a^2}{h^2 m^*}$$

$$E_F = \frac{h^2 m^* a^2}{2 m_e}$$

Unstrained Band Edge Alignment (eV)
(Approximate Alignment to Gold)

