

Slides  
Condensed Matter Physics  
Revision Lecture 1

# HOMEWORKS:

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for commentary

## Problem Set 1

### Einstein, Debye, Drude, and Free Electron Models

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#### 1.1. Einstein Solid

(a) **Classical Einstein Solid (or “Boltzmann” Solid):**

Consider a single harmonic oscillator in three dimensions with Hamiltonian

$$H = \frac{\mathbf{p}^2}{2m} + \frac{k}{2}\mathbf{x}^2$$

▷ Calculate the classical partition function

$$Z = \int \frac{d\mathbf{p}}{(2\pi\hbar)^3} \int d\mathbf{x} e^{-\beta H(\mathbf{p},\mathbf{x})}$$

Note: in this problem  $\mathbf{p}$  and  $\mathbf{x}$  are three dimensional vectors (they should appear bold to indicate this unless your printer is defective).

▷ Using the partition function, calculate the heat capacity  $3k_B$ .

▷ Conclude that if you can consider a solid to consist of  $N$  atoms all in harmonic wells, then the heat capacity should be  $3Nk_B = 3R$ , in agreement with the law of Dulong and Petit.

(b) **Quantum Einstein Solid:** Now consider the same Hamiltonian quantum mechanically.

▷ Calculate the quantum partition function

$$Z = \sum_j e^{-\beta E_j}$$

where the sum over  $j$  is a sum over all Eigenstates.

▷ Explain the relationship with Bose statistics.

▷ Find an expression for the heat capacity.

▷ Show that the high temperature limit agrees with the law of Dulong of Petit.

▷ Sketch the heat capacity as a function of temperature.

The classical calculation has never been on an exam (although it is examinable)

The quantum Einstein model could be on an exam (although it rarely is)

Debye theory is very frequently examined!

## 1.2. Debye Theory:

(a)‡ State the assumptions of the Debye model of heat capacity of a solid.

▷ Derive the Debye heat capacity as a function of temperature (you will have to leave the final result in terms of an integral that cannot be done analytically).

▷ From the final result, obtain the high and low temperature limits of the heat capacity analytically.

You may find the following integral to be useful

$$\int_0^{\infty} dx \frac{x^3}{e^x - 1} = \sum_{n=1}^{\infty} \int_0^{\infty} x^3 e^{-nx} = 6 \sum_{n=1}^{\infty} \frac{1}{n^4} = \frac{\pi^4}{15}$$

By integrating by parts this can also be written as  $\int_0^{\infty} dx \frac{x^4 e^x}{(e^x - 1)^2} = \frac{4\pi^4}{15}$

(b) The following table gives the heat capacity  $C$  for potassium iodide (KI) as a function of temperature.

$T(\text{K})$	0.1	1.0	5	8	10	15	20
$C (\text{J K}^{-1} \text{mol}^{-1})$	$8.5 \times 10^{-7}$	$8.6 \times 10^{-4}$	$1.2 \times 10^{-1}$	$5.9 \times 10^{-1}$	1.1	2.8	6.3

▷ Discuss, with reference to the Debye theory, and make an estimate of the Debye temperature.

### 1.3. Drude Theory of Transport in Metals

Drude theory does show up on exams -- particularly in the context of semiconductors

(a) Assume a scattering time  $\tau$  and use Drude theory to derive an expression for the conductivity of a metal.

(b) Define the resistivity matrix  $\underline{\rho}$  as  $\vec{E} = \underline{\rho}\vec{j}$ .

▷ Use Drude theory to derive an expression for the matrix  $\underline{\rho}$  for a metal in a magnetic field.

(You might find it convenient to assume  $\vec{B}$  parallel to the  $\hat{z}$  axis. The under-tilde notation means that the quantity  $\underline{\rho}$  is a matrix.)

▷ Invert this matrix to obtain an expression for the conductivity matrix  $\underline{\sigma}$ .

(c) Define the Hall coefficient.

▷ Estimate the magnitude of the Hall voltage for a specimen of sodium in the form of a rod of rectangular cross section 5mm by 5mm carrying a current of 1A in a magnetic field of 1T. The density of sodium atoms is roughly 1 gram/cm<sup>3</sup>, and sodium has atomic mass of roughly 23. You may assume that there is one free electron per sodium atom (Sodium has *valence* one).

▷ What practical difficulties would there be in measuring the Hall voltage and resistivity of such a specimen (and how might these difficulties be addressed).

(d) What properties of metals does Drude theory not explain well?

(e)\* Consider now an applied AC field  $\vec{E} \sim e^{i\omega t}$  which induces an AC current  $\vec{j} \sim e^{i\omega t}$ . Modify the above calculation (in the presence of a magnetic field) to obtain an expression for the complex AC conductivity matrix  $\underline{\sigma}(\omega)$ . For simplicity in this case you may assume that the metal is very clean, meaning that  $\tau \rightarrow \infty$ , and you may assume that  $\vec{E} \perp \vec{B}$ . You might again find it convenient to assume  $\vec{B}$  parallel to the  $\hat{z}$  axis. (This problem might look hard, but if you think about it for a bit, it isn't really much harder than what you did above!)

▷ At what frequency is there a divergence in the conductivity?

▷ What does this divergence mean? (When  $\tau$  is finite, the divergence is cut off).

▷ Explain how could one use this divergence (known as the cyclotron resonance) to measure the mass of the electron. ( In fact, in real metals, the measured mass of the electron is generally not equal to the well known value  $m_e = 9.1095 \times 10^{-31}$  kg. This is a result of *band structure* in metals, which we will explain later in the course. )

AC Drude theory is likely to be too hard for an exam

ETC.... SEE MY WEBSITE

# Sample Exams with Solutions:

One on my website

One in back of book

Solutions to 2011 exam on  
web – with all the past papers

PAST PAPERS (1996- present)

Go to my website  
for commentary

## Which Past Paper Questions are on the Syllabus Now?

Condensed Matter Papers 2011,2012. All on Syllabus

B Paper 2010

Q1. On Syllabus. End of part d is tricky and was not really covered, but could be deduced by a perceptive student.

Q 2,3,4,5. On Syllabus.

Q6. Mostly not on syllabus. The students should be able to deduce the density of states of a 2d electron gas.

Q7,8 Not on syllabus

ETC !!!!  
SEE MY WEBSITE!

B Paper 2009.

Q1. On syllabus. This question is solved in great detail in my lecture notes (note also there is an error in the height of data point e of the plot. Discussed in the book)

Q2,3. On syllabus.



# STATISTICAL ANALYSIS OF PAST PAPERS (2004-2012)

Go to my website  
for commentary

**Topic Subtopic**

Year = 04 05 06 07 08 09 10 11 12

**# of Times**

**Something About Phonons**

	<b>9</b>	1	1	1	1	1	1	1	1	1
Define Phonon	1	1								
Phonon Density of States	1						1			
In 2d	1						1			
In 1d / diatomic	1				1					
How would you measure phonons (light/neutrons)	2		1		1					
Why is there a degeneracy of modes at...	2		1					1		
Debye Specific Heat	4		1	1			1			1
Derivation in 3d	2			1						1
Derivation In 2d	2		1				1			
Derivation In 1d	1			1						
How many/ what kind of (acoustic/optical/transverse/longitudinal) phonon	5				1	1	1	1		1
Describe Motion of acoustic/optical modes	4	1			1	1	1			
Some Sort of Harmonic Chain	6		1	1	1	1		1	1	
Diatomic with Two Masses	2				1	1				
Monatomic	2			1						1
Alternating Spring Constants	2		1					1		
monatomic limit of diatomic	2		1			1				
Sketch Dispersions / monatomic diatomic	2	1								1

0

**Something about the Free Electron Gas**

	<b>6</b>		1		1	1	1	1		1
Derive Specific Heat of Fermi Gas	2		1		1					
Define Fermi Energy / Fermi Surface	2					1		1		
Density of States of Free Electron Gas	3		1			1		1		
Definition of	1					1				
Derivation In 3d	1								1	
Derivation In 2d	2		1			0.5		0.5		
Derivation In 1d	0.5							0.5		
Estimate a Fermi Energy / Relationship of N to Ef	4		1		1		1			1

**Topic Subtopic**

**Year = 04 05 06 07 08 09 10 11 12**

**# of Times**

**Something About Diffraction / Crystal Structure**

	04	05	06	07	08	09	10	11	12
Derive Structure Factor / Scattering Amplitude	5	1	1			1		1	1
Calculate Interplanar distances	2		1						1
Diffraction	5	1				1	1	1	1
Derive Systematic Absences	2							1	1
When two atoms scatter same; H not scattering	2			1					1
Analyze a Powder Diffraction Pattern	4	1			1		1		1
Predict Diffraction Data	2			1		1			
Write Down Structure Factor for X	3					1	1		1
Identify a unit cell doubling	2	1	1						
Plan View	2					1		1	
primitive vs conventional unit cell	4			1		1	1	1	
Identify Lattice/Basis	3			1		1			1
Calculate Reciprocal Lattice	2	1	1						
Wigner Seitz / Brillouin Zone Construction	3	1						1	1
Contrast neutron/xray	1						1		
Describe equipment for neutron/xray	2	1	1						

Topic Subtopic	04	05	06	07	08	09	10	11	12
<b>Something about Band Structure/Semiconductor Physics</b>	<b>9</b>	1	1	1	1	1	1	1	1
Nearly Free Electron Model (NFEM)	6			1		1	1	1	1
Derive Gaps of NFEM at zone boundary	3					1		1	1
Draw Dispersion	2						1	1	
Describe Effective Mass	3					1		1	1
Monovalent / Divalent - Metal/Insulator	3					1	1	1	
Gaps open when doubling unit cell	1						1		
Draw a fermi surface in 2d/3d for weak/strong potential	2					1			1
Tight Binding Band	1			1					
Describe Density of States	1			1					
Describe opening of gap	1			1					
Define Effective Mass	3	1				1	1		
Define Chemical Potential / Doping	1					1			
Define Mobility	3	1				1	1		
Define Conductivity	1						1		
Define Hole	1		1						
Signs of velocity, energy, current, ...	1		1						
Law of Mass Action / formula for $n(T, \mu)$	5		1		1	1		1	1
Derivation	4				1	1		1	1
Use to calculate some density/ $\mu$ when doped	4		1		1			1	1
Temperature dependence of semiconductors	2	1				1			
Estimate band gap / doping from data	1					1			
How this would be measured	2	1				1			
How chemical potential changes with doping	1		1						
Density of States (1d, 2d, 3d)	2				0.5	0.5	0.5	0.5	
Optical Properties of Semiconductors	1						1		
Direct / Indirect Gap	1						1		
States bound to donors	1						1		
Drude Theory	1						1		
Derive Hall Coefficient	1						1		
Derive Conductivity/Mobility	2	1					1		
Extract mobility/density from experimental data	1						1		

**Topic Subtopic**

Year = 04 05 06 07 08 09 10 11 12

**# of Times**

<b>Something about magnetism</b>	<b>7</b>	1	1	1	1	1		1	1
Define Para/Diamagnetism	3			1		1		1	
Estimate Larmor Diamagnetism	1			1					
Curie Law Derivation for Spin 1/2	3			1		1		1	
Derive Pauli Paramagnetism	1					1			
Adiabatic Demagnetization	1							1	
What is exchange J	2	1			1				
Molecular (mean) field	5	1	1	1	1				1
Relationship of J to Tc	3		1	1	1				
What causes domains	1	1							
Domain Relation to Hysteresis	2	1			1				
Derive Size of Bloch Wall	1	1							

# The syllabus

## VI: Condensed-matter physics

Free electron model of metals, Fermi energy and Fermi surface. Drude theory, conductivity and Hall effect (one carrier only).

Lattice vibrations: law of Dulong and Petit; phonons; dispersion relation with two atomic types: acoustic and optical branches; Einstein and Debye models of heat capacity.

Structure and types of condensed matter. Bonding of atoms: ionic, covalent, van der Waals, metallic [*Non examinable: hydrogen*]. Elasticity and thermal expansion.

Crystals. Bravais lattices, lattice planes, Miller indices and unit cells (conventional and primitive). Reciprocal lattice: Bragg and Laue formulation of diffraction; Brillouin zone; neutron and x-ray scattering.

Electrons in periodic potentials; tight binding model; band structure; Fermi surface; semiconductors and insulators. Semiconductors: Doping; law of mass action; direct and indirect band gap; concepts of holes and effective mass; mobility and Hall effect in semiconductor [*Non examinable: p-n junction, MOSFET*].

Magnetism: Para-, dia-, ferro-, antiferro-, and ferrimagnetism; application of Hund's rules to determination of magnetic ground states of isolated ions; Local Moment vs Itinerant magnetism. Mean field theory. Domains, domain motion, hysteresis.

# Syllabus Changes:

No Quantum Well

Electrons in periodic potentials; tight binding model; band structure; Fermi surface; semiconductors and insulators. Semiconductors: Doping; law of mass action; direct and indirect band gap; concepts of holes and effective mass; mobility and Hall effect in semiconductor [*Non examinable: p-n junction, MOSFET*].

Magnetism: Para- dia-, ferro-, antiferro-, and ferrimagnetism; application of Hund's rules to determination of magnetic ground states of isolated ions; Local Moment vs Itinerant magnetism. Mean field theory. Domains, domain motion, hysteresis.

No Quenching!

The Long and Short of it...

(giving correct length answers)

New Time Limit = 2 hours!



3. Explain what is meant by the following terms in relation to the electronic bandstructure: *Fermi energy*, *chemical potential*, *Fermi surface* and *effective mass*. [4]

Explain how a weak periodic potential in a (one-dimensional) crystal can lead to the formation of a *band gap*. Sketch and describe qualitatively how the band gap and effective masses close to the Brillouin zone boundaries change as the magnitude of the periodic potential is increased. [8]

A fictitious metal crystallises into a simple cubic lattice with lattice constant  $a$  and one atom per lattice point. The potential in the crystal is weakly modulated with the periodicity of the lattice. Sketch the first Brillouin zone for this crystal. The metal is monovalent (that is, it has only one valence electron per unit cell). Describe the shape and dimensions of the Fermi surface if the modulation is extremely weak. What if it is somewhat weak (compared to the Fermi energy), but not extremely weak? A second metal has an identical unit cell, but is divalent (two valence electrons per unit cell). Give a qualitative description and sketch of the Fermi surface for this divalent metal. Discuss what happens in both the monovalent and divalent cases as the periodic potential becomes extremely strong. [8]

From Collection (2008 Exam)

5. Explain briefly the origin of the electronic band gap in a typical electrical insulator.

[6]

The periodic potential  $V(x)$  experienced by an electron in a one-dimensional crystal may be given in the form

$$V(x) = V_0 + V_G e^{-iGx} + V_{-G} e^{+iGx},$$

where  $G$  is the reciprocal lattice vector, and  $|V_G| = |V_{-G}|$ . Explain why a suitable wavefunction for an electron in such a potential may be written to a first approximation as

$$\psi(x) = Ae^{ikx} + Be^{i(k-G)x}.$$

[3]

By substituting  $\psi(x)$  into the Schrödinger equation and comparing coefficients in  $e^{ikx}$  and  $e^{i(k-G)x}$ , show that the energy of an electron of mass  $m$  and wavevector  $k$  at the zone boundary is given by

$$E = V_0 + \frac{\hbar^2 k^2}{2m} \pm |V_G|.$$

Discuss the significance of each of the three terms on the right-hand side of this equation in terms of band theory.

[10]

Using this result explain why diamond is a good electrical insulator, whereas silicon and germanium, which have the same structure type as diamond, are semiconductors. (In the diamond structure there are two tetravalent atoms in the basis.)

[6]

# Some Random Comments

## Phase velocities in the 1D chain

Posted by Another Shrugging Physicist on February 1, 2013, 6:01 pm

In lectures we derived the dispersion relation for the 1D monatomic chain as  $\omega \sim |\sin(ka/2)|$ . That could be defined as having a Brillouin zone as either between  $-\pi/a$  and  $\pi/a$  or  $0$  and  $2\pi/a$ , and it is exactly equivalent in either, as it should be.

**But what about the phase velocity  $\omega/k$ ?** If we use the first definition of the Brillouin zone we'll have a large (negative) value of the velocity just below zero, as it's roughly a sinc function, but if we use the second definition in the equivalent place (just below  $2\pi/a$ ) we'll have a tiny phase velocity. The first one seems more realistic, but shouldn't these be reproducing exactly the same physics?

## Crystal Momentum

Posted by Steve Simon on January 31, 2013, 2:52 pm

A good question was asked today after lecture:

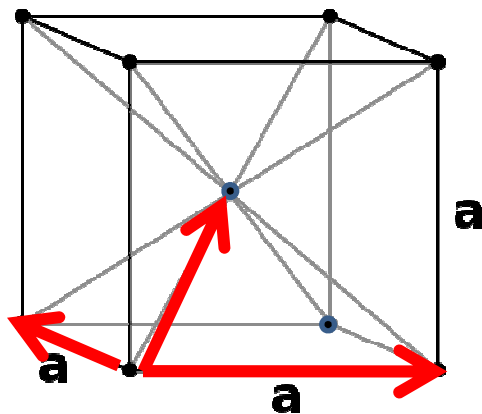
Q: If  $k$  is a wavevector, we usually think of  $2\pi/k$  as being the wavelength. What does it then mean that  $k$  is the same as  $k + 2\pi/a$  as we found for the vibrational waves and the tight binding chain?



## 6.6. Reciprocal Lattice

Show that the reciprocal lattice of a FCC (face-centered-cubic) lattice is a BCC (body-centered-cubic) lattice. Correspondingly show that the reciprocal lattice of a BCC lattice is an FCC lattice. If an FCC lattice has conventional unit cell with lattice constant  $a$ , what is the lattice constant for the conventional unit cell of the reciprocal BCC lattice?

BCC



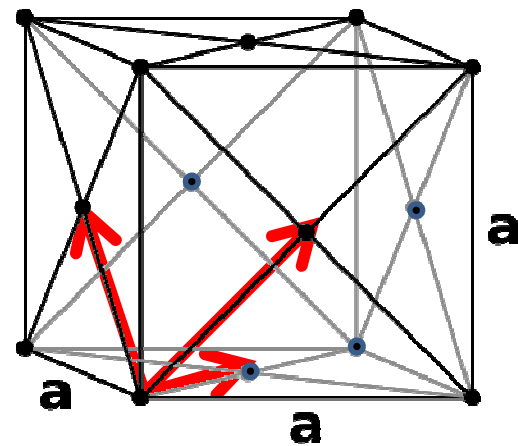
Primitive lattice vectors

$$\mathbf{a}_1 = [1, 0, 0] a$$

$$\mathbf{a}_2 = [0, 1, 0] a$$

$$\mathbf{a}_3 = [\frac{1}{2}, \frac{1}{2}, \frac{1}{2}] a$$

FCC



Primitive lattice vectors

$$\mathbf{a}_1 = [\frac{1}{2}, \frac{1}{2}, 0] a$$

$$\mathbf{a}_2 = [0, \frac{1}{2}, \frac{1}{2}] a$$

$$\mathbf{a}_3 = [\frac{1}{2}, 0, \frac{1}{2}] a$$

Tomorrow (Tentative):

Some stuff about Magnetism

Question 7 from 2011 exam (Band gaps etc)

First question from the collection (2008 exam)

Other suggestions?

(tell me now!)