Slides
Condensed Matter Physics
Revision Lecture 1

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Problem Set 1

Einstein, Debye, Drude, and Free Electron Models

1.1. **Einstein Solid**

Classical Einstein Solid (or "Boltzmann" Solid): Consider a single harmonic oscillator in three dimensions with Hamiltonian

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

The classical calculation has never been examined on the condensed matter exam

Calculate the classical partition function

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

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.

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.

(See also problem A.1.1. for more on the same topic)

1.2. **Debye Theory:**

Debye theory is examined frequently!

(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.

(b) The following table gives the heat capacity C for KCl as a function of temperature. Discuss, with reference to the Debye theory, and make an estimate of the Debye temperature.

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

For part (a) you may find the following integral to be useful

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

Alternately, you may find useful the form

$$\int_0^\infty dx \frac{x^4 e^x}{(e^x - 1)^2} = \frac{4\pi^4}{15}$$

which you can derive from the first by integrating by parts.

Basic Drude theory has been examined lots. Make sure to know how it works for semiconductors too.

Finite frequency Drude is probably too hard for an exam

1.3. Drude Theory of Transport in Metals

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

(b)Define the resistivity matrix $\underset{\sim}{\rho}$ as $\vec{E} = \underset{\sim}{\rho}\vec{j}$. Use Drude theory to derive an expression for the matrix $\underset{\sim}{\rho}$ for a metal in a magnetic field. (You might find it convenient to assume $\vec{B}$ parallel to the $\hat{z}$ axis.) Invert this matrix to obtain an expression for the conductivity tensor.

(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^3, and sodium has atomic mass of roughly 23. What practical difficulties would there be in measuring the Hall voltage and resistivity of such a specimen (and how might these difficulties be addressed). You may assume that there is one free electron per sodium atom (Sodium has *valence* one).

(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 $\underset{\sim}{\sigma}(\omega)$. For simplicity in this case you may assume that the metal is very clean, meaning that $\tau \to \infty$, 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.) At what frequency is there a divergence in the conductivity? What does this divergence mean? (When τ 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.)

ETC.... SEE MY WEBSITE

PAST PAPERS (1996-2010)

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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.

Q2. On Syllabus. The [7] point part is tricky

Q3. On Syllabus.

Q4. On Syllabus, although for part b we have only discussed effective masses at the extrema of the bands.

Q5. On syllabus.

Q6. The first two parts are mostly on syllabus, although we covered them only very briefly. The final part about constructing a laser is certainly not. The students should be able to deduce the density of states of a 2d electron gas. Figuring out how the multiple states in a quantum well change this density of states would require some thinking and was not covered (but clever students might get it).

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 my lecture notes page 136)

Q2. On syllabus.

Q3. On syllabus.

Q4. On syllabus. We did not explicitly discuss part (c) but a clever student should be able to figure it out.

Q6. As with Q6 of 2010, this is mostly on syllabus except the last part discussing lasers. The students should be able to derive the density of states in 1d. Again, figuring out how the multiple states in a quantum well change this density of states would require some thinking and was not covered (but clever students might get it).

ETC !!!!
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STATISTICAL ANALYSIS OF PAST PAPERS (2004-2010)

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Topic Subtopic	Year = # of Times	04	05	06	07	08	09	10
Something About Phonons	7	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…	1		1					
Debye Specific Heat	3		1	1			1	
Derivation in 3d	1			1				
Derivation In 2d	2		1				1	
Derivation In 1d	1			1				
How many/ what kind of (acoustic/optical/transverse/longitudinal) phonon	4				1	1	1	1
Describe Motion of acoustic/optical modes	4	1			1	1	1	
Some Sort of Harmonic Chain	5		1	1	1	1		1
Diatomic with Two Masses	2				1	1		
Monatomic	1			1				
Alternating Sprint Constants	2		1					1
monatomic limit of diatomic	2		1			1		
Sketch Dispersions / monotomic diatomic	1	1						
Something about the Free Electron Gas	5		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			1		0.5
Derivation In 1d	0.5						0.5	
Estimate a Fermi Energy / Relationship of N to Ef	3		1		1		1	

Topic Subtopic	Year = # of Times	04	05	06	07	08	09	10
Something About Diffraction / Crystal Structure	7	1	1	1	1	1	1	1
Derive Structure Factor / Scattering Amplitude	4	1	1			1		1
Calculate Interplanar distances	1		1					
Diffraction	4	1				1	1	1
Derive Systematic Absences	1							1
When two atoms scatter same; H not scattering	1			1				
Analyze a Powder Diffraction Pattern	3	1			1		1	
Predict Diffraction Data	2			1		1		
Write Down Structure Factor for X	2					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	2			1		1		
Calculate Reciprocal Lattice	2	1	1					
Wigner Seitz / Brillouin Zone Construction	2	1						1
Contrast neutron/xray	1						1	
Describe equipment for neutron/xray	2	1	1					

Topic	Subtopic	Year = # of Times	04	05	06	07	08	09	10
Something about Band Structure/Semicondcuctor Physics		7	1	1	1	1	1	1	1
Nearly Free Electron Model (NFEM)		4			1		1	1	1
	Derive Gaps of NFEM at zone boundary	2					1		1
	Draw Dispersion	2						1	1
	Describe Effective Mass	2					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	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)		4		1		1	1		1
	Derivation	3				1	1		1
	Use to calculate some density/mu when doped	3		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					
Quantum Well		2.5			0.5	0.5	1	0.5	0.5
	Density of States in 2d	1.5				0.5	1		0.5
	Density of States In 1d	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 = # of Times	04	05	06	07	08	09	10
Something about magnetism	6	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	4	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						

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

$$V(x) = V_0 + V_G\,\mathrm{e}^{-\mathrm{i}Gx} + V_{-G}\,\mathrm{e}^{+\mathrm{i}Gx},$$

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

$$\psi(x) = A\mathrm{e}^{\mathrm{i}kx} + B\mathrm{e}^{\mathrm{i}(k-G)x}.$$ [3]

By substituting $\psi(x)$ into the Schrödinger equation and comparing coefficients in $\mathrm{e}^{\mathrm{i}kx}$ and $\mathrm{e}^{\mathrm{i}(k-G)x}$, 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]