# Problems for Solid State Physics
# (3rd Year Course 6)
# Hilary Term 2012

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"Everything should be made as simple as possible, but no simpler."

— Frequently attributed to Albert Einstein

Actual quote:

"It can scarcely be denied that the supreme goal of all theory is to make the irreducible basic elements as simple and as few as possible without having to surrender the adequate representation of a single datum of experience"

— Albert Einstein, lecture delivered at Oxford 10 June 1933

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‡ Denotes crucial problems that you need to be able to do in your sleep.
* Denotes problems that are slightly harder.

Annotations of Homeworks 2012

-- including which topics are the most important to study for the exam!

Much of this problem set is standard exam material.

# 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

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

the classical calculation has never been on the condensed matter exam (although it is examinable)

▷ Calculate the classical partition function

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

Note: in this problem **p** and **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

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

The quantum Einstein model could be on the exam (albeit rarely)

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:

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

Debye Model is very frequently examined!

▷ 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 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 $^{-1}$) | $8.5\times10^{-7}$ | $8.6\times10^{-4}$ | $1.2\times10^{-1}$ | $5.9\times10^{-1}$ | 1.1 | 2.8 | 6.3 |

### 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 $\underset{\sim}{\rho}$ as $\vec{E} = \underset{\sim}{\rho}\vec{j}$.

$\triangleright$ 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. The under-tilde notation means that the quantity $\underset{\sim}{\rho}$ is a matrix.)

$\triangleright$ Invert this matrix to obtain an expression for the conductivity matrix $\underset{\sim}{\sigma}$.

(c) Define the Hall coefficient.

$\triangleright$ 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. You may assume that there is one free electron per sodium atom (Sodium has *valence* one).

$\triangleright$ 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?

AC Drude theory is probably too hard for an exam.

(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. (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!)

$\triangleright$ At what frequency is there a divergence in the conductivity?

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

$\triangleright$ 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 $m_e = 9.1095\times10^{-31}$ kg. This is a result of *band structure* in metals, which we will explain later in the course. )

### 1.4. Fermi Surface in the Free Electron (Sommerfeld) Theory of Metals

This is a standard exam question

(a)‡ Explain what is meant by the Fermi energy, Fermi temperature and the Fermi surface of a metal.

(b)‡ Obtain an expression for the Fermi wavevector and the Fermi energy for a gas of electrons (in 3D).

$\triangleright$ Show that the density of states at the Fermi surface, $dN/dE_F$ can be written as $3N/2E_F$.

(c) Estimate the value of $E_F$ for sodium [As above, the density of sodium atoms is roughly 1 gram/cm$^3$, and sodium has atomic mass of roughly 23. You may assume that there is one free electron per sodium atom (Sodium has *valence* one)]

(d) Now consider a two dimensional Fermi gas. Obtain an expression for the density of states at the Fermi surface.

### 1.5. Velocities in the Free Electron Theory

Also a standard exam question

(a) Assuming that the free electron theory is applicable: show that the speed $v_F$ of an electron at the Fermi surface of a metal is $v_F = \frac{\hbar}{m}(3\pi^2 n)^{1/3}$ where $n$ is the density of electrons.

(b) Show that the mean drift speed $v_d$ of an electron in an applied electric field $E$ is $v_d = |\sigma E/(ne)|$, where $\sigma$ is the electrical conductivity, and show that $\sigma$ is given in terms of the mean free path $\lambda$ of the electrons by $\sigma = ne^2\lambda/(mv_F)$.

(c) Assuming that the free electron theory is applicable to copper:

(i) calculate the values of both $v_d$ and $v_F$ for copper at 300K in an electric field of 1 V $\text{m}^{-1}$ and comment on their relative magnitudes.

(ii) estimate $\lambda$ for copper at 300K and comment upon its value compared to the mean spacing between the copper atoms.

Copper is monovalent, meaning there is one free electron per atom. The density of atoms in copper is $n = 8.45 \times 10^{28}$ $\text{m}^{-3}$. The conductivity of copper is $\sigma = 5.9 \times 10^7 \Omega^{-1}\text{m}^{-1}$ at 300K.

### 1.6. Physical Properties of the Free Electron Gas

Also very standard exam question

In both (a) and (b) you may always assume that the temperature is much less than the Fermi temperature.

(a)‡ Give a simple but approximate derivation of the Fermi gas prediction for heat capacity of the conduction electron in metals

(b)‡ Give a simple (not approximate) derivation of the Fermi gas prediction for magnetic susceptibility of the conduction electron in metals. Here susceptibility is $\chi = dM/dH = \mu_0 dM/dB$ at small $H$ and is meant to consider the magnetization of the electron spins only.

(c) How are the results of (a) and (b) different from that of a classical gas of electrons?

▷ What other properties of metals may be different from the classical prediction?

(d) The experimental heat capacity of potassium metal at low temperatures has the form:

$$C = (2.08\,T + 2.6\,T^3)\text{mJ}\,\text{mol}^{-1}\,\text{K}^{-1}$$

where $T$ is in Kelvin.

▷ Explain the origin of each of the two terms in this expression.

▷ Make an estimate of the Fermi energy for potassium metal.

This problem set has a lot of material which, while in principle examinable, is not likely to show up. The last two problems on this set are very very important though.

# Problem Set 2

Chemical Bonding, Thermal Expansion, Normal Modes, Phonons in 1d

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Chemical bonding is mandated by IOP. It has never been examined in a condensed matter exam as far as I know. Although examinable it would be a departure from tradition

## 2.1. Chemical Bonding

(a) Qualitatively describe five different types of chemical bonds and why they occur.

▷ Describe which combinations of what types of atoms are expected to form which types of bonds (make reference to location on the periodic table).

▷ Describe some of the qualitative properties of materials that have these types of bonds.

(Yes, you can just copy the table out of the notes, but the point of this exercise is to learn the information in the table!)

(b) Describe qualitatively the phenomenon of Van der Waals forces. Explain why the force is attractive and proportional to $1/R^7$ where $R$ is the distance between two atoms.

Similarly, covalent bonding is mandated by IOP but has never been examined.

## 2.2. Covalent Bonding in Detail*

(a) **Linear Combination of Atomic Orbitals (LCAO)** In class we considered two atoms each with a single atomic orbital. We called the orbital $|1\rangle$ around nucleus 1 and $|2\rangle$ around nucleus 2. More generally we may consider any set of wavefunctions $|n\rangle$ for $n = 1, \ldots, N$. For simplicity, let us assume this basis is orthonormal $\langle n|m\rangle = \delta_{n,m}$

Let us write a trial wavefunction for our ground state as

$$|\Psi\rangle = \sum_n \phi_n |n\rangle$$

This is known as a linear combination of atomic orbitals (LCAO). We would like to find the lowest energy wavefunction we can construct in this form, that is the best approximation to the actual ground state wavefunction. (The more states we use in our basis, generally, the more accurate our results will be).

We claim that the the ground state is given by the solution of the effective Schroedinger equation

$$\mathcal{H}\,\boldsymbol{\phi} = E\,\boldsymbol{\phi} \tag{1}$$

where $\boldsymbol{\phi}$ is the vector of $N$ coefficients $\phi_n$, and $\mathcal{H}$ is the $N$ by $N$ matrix

$$\mathcal{H}_{n,m} = \langle n|H|m\rangle$$

with $H$ the Hamiltonian of the full system we are considering.

To prove this, let us construct the energy

$$E = \frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle}$$

▷ Show that minimizing this energy with respect to each $\phi_n$ gives the same eigenvalue equation, Eq. 1. (Caution: $\phi_n$ is generally complex! If you are not comfortable with complex differentiation, write everything in terms of real and imaginary parts of each $\phi_n$). Similarly, the second eigenvalue of the effective Schroedinger equation will be an approximation to the first excited state of the system.

This technique is know as the molecular orbital approach, or the LCAO (linear combination of atomic orbitals) approach. It is used heavily in numerical simulation of molecules. However, more generally, one cannot assume that the basis set of orbitals is orthonormal. In problem A.2.1. we properly consider a non-orthonormal basis.

I think you have to know something about this for your atomic paper anyway

(b) **Two-orbital covalent bond** Let us return to the case where there are only two orbitals in our basis. This pertains to a case where we have two identical nuclei and a single electron which will be shared between them to form a covalent bond. We write the full Hamiltonian as

$$H = \frac{\mathbf{p}^2}{2m} + V(\mathbf{r} - \mathbf{R_1}) + V(\mathbf{r} - \mathbf{R_2}) = K + V_1 + V_2$$

where $V$ is the Coulomb interaction between the electron and the nucleus, $R_1$ is the position of the first nucleus and $R_2$ is the position of the second nucleus. Let $\epsilon$ be the energy of the atomic orbital around one nucleus in the absence of the other. In other words

$$\begin{aligned} (K + V_1)|1\rangle &= \epsilon|1\rangle \\ (K + V_2)|2\rangle &= \epsilon|2\rangle \end{aligned}$$

Define also the cross-energy element

$$V_{cross} = \langle 1|V_2|1\rangle = \langle 2|V_1|2\rangle$$

and the hopping matrix element

$$t = -\langle 1|V_2|2\rangle = -\langle 1|V_1|2\rangle$$

These are not typos!

▷ Why can we write $V_{cross}$ and $t$ equivalently using either one of the expressions given on the right hand side?

▷ Show that the eigenvalues of our Schroedinger equation Eq. 1 are given by

$$E = \epsilon + V_{cross} \pm |t|$$

▷ Argue (perhaps using Gauss's law) that $V_{cross}$ should roughly cancel the repulsion between nuclei, so that, in the lower eigenstate the total energy is indeed lower when the atoms are closer together.

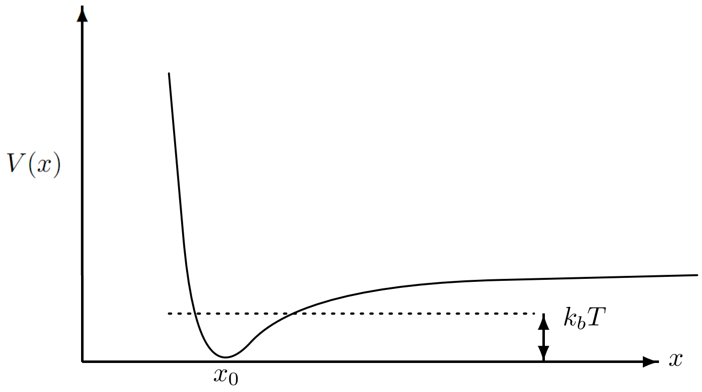
▷ This approximation must fail when the atoms get sufficiently close. Why?

### 2.3. Thermal Expansion

As a model of thermal expansion, we study the distance between two nearest neighbor atoms in an anharmonic potential that looks roughly like this

Thermal expansion is also mandated by IOP, but has never been examined.

I think it would be unlikely to show up.



where $x$ is the distance between the two neighboring atoms. This potential can be expanded around its minimum as

$$V(x) = \frac{\kappa}{2}(x-x_0)^2 - \frac{\kappa_3}{3!}(x-x_0)^3 + \ldots \tag{2}$$

where the minimum is at position $x_0$ and $\kappa_3 > 0$. For small energies, we can truncate the series at the cubic term.

(a) A very accurate approximate form for inter-atomic potentials (particularly for inert atoms such as Helium or Argon) is given by the so-called Lennard-Jones potential

Lennard-Jones Potential
Showed up last year!

$$V(x) = 4\epsilon\left[\left(\frac{\sigma}{x}\right)^{12} - \left(\frac{\sigma}{x}\right)^{6}\right] \tag{3}$$

where $\epsilon$ and $\sigma$ are constants that depend on the particular atoms we are considering.

▷ What is the meaning of the exponent 6 in the second term of this expression. (i.e., why is the exponent necessarily chosen to be 6).

▷ By expanding Eq. 3 around its minimum, and comparing to Eq. 2, calculate the values of the coefficients $x_0$, $\kappa$, and $\kappa_3$ for the Lennard-Jones potential in terms of the constants $\epsilon$ and $\sigma$. We will need these results below.

(b) **Classical model:**

(i) In classical statistical mechanics, we write the expectation of $x$ as

$$\langle x\rangle_\beta = \frac{\int dx\, x\, e^{-\beta V(x)}}{\int dx\, e^{-\beta V(x)}}$$

Although one cannot generally do such integrals for arbitrary potential $V(x)$ as in Eq. 2, one can expand the exponentials as

$$e^{-\beta V(x)} = e^{-\frac{\beta\kappa}{2}(x-x_0)^2}\left[1 + \frac{\beta\kappa_3}{6}(x-x_0)^3 + \ldots\right]$$

and let limits of integration go to $\pm\infty$

▷ Why is this expansion of the exponent and the extension of the limits of integration allowed?

▷ Use this expansion to derive $\langle x\rangle_\beta$ to lowest order in $\kappa_3$, and hence show that the coefficient of thermal expansion is

$$\alpha = \frac{1}{L}\frac{dL}{dT} \approx \frac{1}{x_0}\frac{d\langle x\rangle_\beta}{dT} = \frac{1}{x_0}\frac{k_b\,\kappa_3}{2\kappa^2}$$

with $k_b$ Boltzmann's constant.

▷ In what temperature range is the above expansion valid?

(ii) For Argon, the the Lennard-Jones constants $\epsilon$ from Eq. 3 is given by $\epsilon = 10\text{meV}$

▷ Estimate the thermal expansion coefficient $\alpha$ of Argon. Note: *You can do this part even if you got stuck on some of the above parts!*

The actual thermal expansion coefficient of Argon is approximately $\alpha = 2\times10^{-3}/\text{K}$ at about 80 K. However at lower temperature $\alpha$ drops quickly. We will use a more sophisticated quantum model to understand why this is so.

(iii) While this model of thermal expansion in a solid is valid if there are only two atoms, why is it invalid for the case of a many-atom chain? (Although it is not so bad as an approximation!)

Quantum model is way too hard for an exam.

(c) **Quantum model:**

(i) In quantum mechanics we write a Hamiltonian

$$H = H_0 + V$$

where

$$H_0 = \frac{p^2}{2m} + \frac{\kappa}{2}(x - x_0)^2 \qquad (4)$$

is the Hamiltonian for the free Harmonic oscillator, and $V$ is the perturbation

$$V = -\frac{\kappa_3}{6}(x - x_0)^3 + \ldots$$

where we will throw out quartic and higher terms.

▷ What value of $m$ should be used in Eq. 4?

Using perturbation theory it can be shown that, to lowest order in $\kappa_3$ the following equation holds

$$\langle n|x|n\rangle = x_0 + E_n \kappa_3/(2\kappa^2) \qquad (5)$$

where $|n\rangle$ is the eigenstate of the Harmonic oscillator whose energy is

$$E_n = \hbar\omega(n + \frac{1}{2}) + \mathcal{O}(\kappa_3) \qquad n \geq 0$$

with $\omega = \sqrt{\kappa/m}$. In (iii) below we will prove Eq. 5. For now, take it as given.

▷ Note that even when the oscillator is in its ground state, the expectation of $x$ deviates from $x_0$. Physically why is this?

(ii)* Use, Eq. 5 to calculate the quantum expectation of $x$ at any temperature. We write

$$\langle x\rangle_\beta = \frac{\sum_n \langle n|x|n\rangle e^{-\beta E_n}}{\sum_n e^{-\beta E_n}}$$

▷ Derive the coefficient of thermal expansion.

▷ Examine the high temperature limit and show that it matches that of part $b$ above.

▷ In what range of temperatures is our perturbation expansion valid?

▷ In light of the current quantum calculation, when is the above classical calculation valid?

▷ Why does the thermal expansion coefficient drop at low temperature.

(iii)** Prove Eq. 5 above by using lowest order perturbation theory.

It is easiest to perform this calculation by using raising and lowering (ladder) operators. Recall that one can define operators $a$ and $a^\dagger$ such that $[a, a^\dagger] = 1$ and

$$\begin{aligned} a^\dagger|n\rangle &= \sqrt{n+1}|n+1\rangle \\ a|n\rangle &= \sqrt{n}|n-1\rangle \end{aligned}$$

In terms of these operators, we have the operator $x - x_0$ given by

$$x - x_0 = \sqrt{\frac{\hbar}{2m\omega}}(a + a^\dagger)$$

### 2.4. Classical Normal Modes to Quantum Eigenstates

This has never been on an exam.

I wrote a rant last year about how I'd love to see something like this on an exam because it is fundamental to the idea of a phonon But I think it would be a fairly large departure from tradition.

In class we stated, without proof that a classical normal mode becomes a quantum eigenstate. Here we prove this fact for a simple diatomic molecule in a potential well. (See also problem A.1.1.)

Consider two particles, each of mass $m$ in one dimension, connected by a spring ($K$), at the bottom of a potential well (with spring constant $k$). We write the potential energy as

$$U = \frac{k}{2}(x_1^2 + x_2^2) + \frac{K}{2}(x_1 - x_2)^2$$

▷ Write the classical equations of motion.

▷ Transform into relative $x_{rel} = (x_1 - x_2)$ and center of mass $x_{cm} = (x_1 + x_2)/2$ coordinates.

(a) Show that in these transformed coordinates, the system decouples, thus showing that the two normal modes have frequencies

$$\begin{aligned} \omega_{cm} &= \sqrt{k/m} \\ \omega_{rel} &= \sqrt{(k+2K)/m} \end{aligned}$$

Note that since there are two initial degrees of freedom, there are two normal modes.

Now consider the quantum mechanical version of the same problem. The Hamiltonian is

$$H = \frac{p_1^2}{2m} + \frac{p_2^2}{2m} + U(x_1, x_2)$$

▷ Again transform into relative and center of mass coordinates.

Define the corresponding momenta are given by $p_{rel} = (p_1 - p_2)/2$ and $p_{cm} = (p_1 + p_2)$.

(b) Show that $[p_\alpha, x_\gamma] = -i\hbar\delta_{\alpha,\gamma}$ where $\alpha$ and $\gamma$ take the values $cm$ or $rel$.

(c) In terms of these new coordinates show that the Hamiltonian decouples into two independent harmonic oscillators with the same eigenfrequencies $\omega_{cm}$ and $\omega_{rel}$. Conclude that the spectrum of this system is

$$E_{n_{rel}, n_{cm}} = \hbar\omega_{rel}(n_{rel} + \frac{1}{2}) + \hbar\omega_{cm}(n_{cm} + \frac{1}{2})$$

where $n_{cm}$ and $n_{rel}$ are nonnegative integers.

(d) At temperature $T$ what is the expectation of the energy of this system?

In problem A.2.4. the principle that normal modes become quantum eigenstates is proven in more generality.

### 2.5. Normal Modes of a One Dimensional Monatomic Chain

This is SUPER important.

Know this stuff inside out.

It shows up almost every year.

(a)‡ Explain what is meant by "normal mode" and by "phonon".

▷ Explain briefly why phonons obey Bose statistics.

(b)‡ Derive the dispersion relation for the longitudinal oscillations of a one dimensional mass-and-spring crystal with $N$ identical atoms of mass $m$, lattice spacing $a$, and spring constant $\kappa$. (Motion of the masses is restricted to be in one dimension).

(c)‡ Show that the mode with wavevector $k$ has the same pattern of mass displacements as the the mode with wavevector $k + 2\pi/a$. Hence show that the dispersion relation is periodic in reciprocal space ($k$-space).

▷ How many *different* normal modes are there.

(d)‡ Derive the phase and group velocities and sketch them as a function of $k$.

▷ What is the sound velocity?

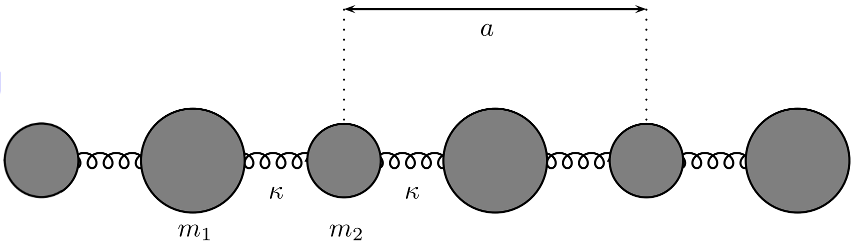
▷ Show that the the sound velocity is also given by $v_s = \sqrt{\beta^{-1}/\rho}$ where $\rho$ is the chain density and $\beta$ is the compressibility.

(e) Find the expression for $g(\omega)$, the density of states of modes per angular frequency.

▷ Sketch $g(\omega)$.

### 2.6. Normal modes of a One Dimensional Diatomic Chain*

**Also SUPER important. You should know both the case of alternating masses and alternating spring constants. (we did the latter in lecture).**



(a) What is the difference between an acoustic mode and an optical mode.

▷ Describe how particles move in each case.

(b) Derive the dispersion relation for the longitudinal oscillations of a one dimensional *diatomic* mass-and-spring crystal where the unit cell is of length $a$ and each unit cell contains one atom of mass $m_1$ and one atom of mass $m_2$ connected together by springs with spring constant $\kappa$ (all springs are the same, and motion of particles is in one dimension only).

(c) Determine the frequencies of the acoustic and optical modes at $k = 0$ as well as at the Brillouin zone boundary.

▷ Determine the sound velocity and show that the group velocity is zero at the zone boundary.

▷ Show that the the sound velocity is also given by $v_s = \sqrt{\beta^{-1}/\rho}$ where $\rho$ is the chain density and $\beta$ is the compressibility.

(d) Sketch the dispersion in both reduced and extended zone scheme.

▷ If there are $N$ unit cells, how many different normal modes are there?

▷ How many *branches* of excitations are there? (I.e., in reduced zone scheme, how many modes are there there at each $k$).

(e) What happens when $m_1 = m_2$ ?

### 2.7. One more problem

Problem 3.8. really belongs to this problem set, but this set is too long already, so I pushed it to the next problem set. If you have extra time, give it a shot.

**You can be almost guaranteed that there will be an exam question on crystal structure and/or scattering.**

# Problem Set 3

Crystal Structure, Reciprocal Lattice, and Scattering (plus tightbinding in 1d tacked on)

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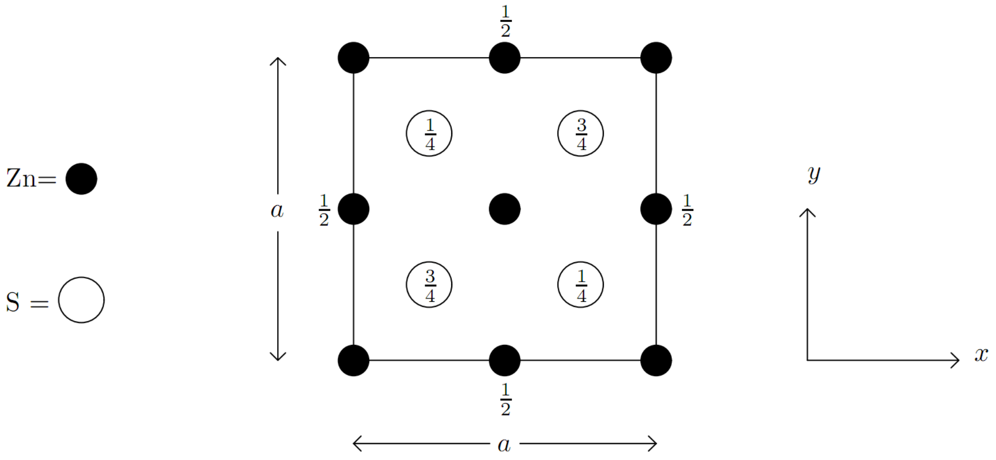
### 3.1. Crystal Structure

**This is a very standard exam question. Know how to do this!**



The diagram above shows a plan view of a structure of cubic ZnS (zinc blende) looking down the $z$ axis. The numbers attached to some atoms represent the heights of the atoms above the $z = 0$ plane expressed as a fraction of the cube edge $a$. Unlabeled atoms are at $z = 0$ and $z = a$.

(a) What is the Bravais lattice type

(b) Describe the basis

(c) Given that $a = 0.541$ nm, calculate the nearest-neighbor Zn-Zn, Zn-S, and S-S distances.

(d) Copy the drawing above, and show the [210] direction and the set of (210) planes.

(e) Calculate the spacing between adjacent (210) planes.

### 3.2. Directions and Spacings of Crystal Planes

**Also very standard exam question**

▷ Explain briefly what is meant by the terms “Crystal Planes” and “Miller Indices” for the case where the axes of a lattice are all mutually orthogonal to each other.

▷ Show that the general direction $[hkl]$ in a cubic crystal is normal to the planes with Miller indices $(hkl)$.

▷ Is the same true in general for an orthorhombic crystal?

▷ Show that the spacing $d$ of the $(hkl)$ set of planes in a cubic crystal with lattice parameter $a$ is

$$d = \frac{a}{\sqrt{h^2 + k^2 + l^2}}$$

▷ What is the generalization of this formula for an orthorhombic crystal?

### 3.3. ‡Reciprocal Lattice

**Same. Know this!**

(a) Define the term Reciprocal Lattice.

(b) Show that if a lattice in 3d has primitive lattice vectors $\mathbf{a_1}$, $\mathbf{a_2}$ and $\mathbf{a_3}$ then primitive lattice vectors for the reciprocal lattice can be taken as

$$\begin{aligned} \mathbf{b_1} &= 2\pi \frac{\mathbf{a_2} \times \mathbf{a_3}}{\mathbf{a_1} \cdot (\mathbf{a_2} \times \mathbf{a_3})} && (1) \\ \mathbf{b_2} &= 2\pi \frac{\mathbf{a_3} \times \mathbf{a_1}}{\mathbf{a_1} \cdot (\mathbf{a_2} \times \mathbf{a_3})} && (2) \\ \mathbf{b_3} &= 2\pi \frac{\mathbf{a_1} \times \mathbf{a_2}}{\mathbf{a_1} \cdot (\mathbf{a_2} \times \mathbf{a_3})} && (3) \end{aligned}$$

What is the proper formula in 2d?

(c) Define tetragonal and orthorhombic lattices. For an orthorhombic lattice, show that $|\mathbf{b_j}| = 2\pi/|\mathbf{a_j}|$. Hence, show that the length of the reciprocal lattice vector $\mathbf{G} = h\mathbf{b_1} + k\mathbf{b_2} + l\mathbf{b_3}$ is equal to $2\pi/d$, where $d$ is the spacing of the $(hkl)$ planes (see question 3.2.)

Know this

### 3.4. Reciprocal Lattice and X-ray Scattering

A two-dimensional rectangular crystal has a unit cell with sides $a_1 = 0.468$ nm and $a_2 = 0.342$ nm. A collimated beam of monochromatic X-rays with wavelength 0.166 nm is used to examine the crystal.

(a) Draw to scale a diagram of the reciprocal lattice.

▷ Label the reciprocal lattice points for indices in the range $0 \le h \le 3$ and $0 \le k \le 3$.

(b) Calculate the magnitude of the wavevectors $\mathbf{k}$ and $\mathbf{k}'$ of the incident and reflected X-ray beams, and hence construct on your drawing the "scattering triangle" corresponding to the Laue condition $\Delta\mathbf{k} = \mathbf{G}$ for diffraction from the (210) planes. (the scattering triangle includes $\mathbf{k}$, $\mathbf{k}'$ and $\Delta\mathbf{k}$).

(c) Draw the first and second Brillouin zones using the Wigner-Seitz construction.

Know this too!

### 3.5. ‡ X-ray scattering II

$BaTiO_3$ has a primitive cubic lattice and a basis with atoms having fractional coordinates

| | | | |
|---|---|---|---|
| Ba | (0,0,0) | | |
| Ti | $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ | | |
| O | $(\frac{1}{2}, \frac{1}{2}, 0)$, | $(\frac{1}{2}, 0, \frac{1}{2})$, | $(0, \frac{1}{2}, \frac{1}{2})$ |

▷ Sketch the unit cell.

▷ Show that the X-ray structure factor for the $(00l)$ Bragg reflections is given by

$$S_{hkl} = f_{Ba} + (-1)^l f_{Ti} + \left[1 + 2(-1)^l\right] f_O \tag{4}$$

where $f_{\mathrm{Ba}}$ is the atomic form factor for Ba, etc.

▷ Calculate the ratio $I_{002}/I_{001}$, where $I_{hkl}$ is the intensity of the X-ray diffraction from the $(hkl)$ planes. You may assume that the atomic form factor is proportional to atomic number $(Z)$, and neglect its dependence on the scattering vector. [ $Z_{\mathrm{Ba}} = 56$, $Z_{\mathrm{Ti}} = 22$, $Z_{\mathrm{O}} = 8$ ]

Also standard
exam question

### 3.6. ‡ X-ray scattering and Systematic Absences

(a) Explain what is meant by "Lattice Constant" for a cubic crystal structure.

(b) Explain why X-ray diffraction may be observed in first order from the (110) planes of a crystal with a body-centred cubic lattice, but not from the (110) planes of a crystal with a face-centred cubic lattice.

▷ Derive the general selection rules for which planes are observed in bcc and fcc lattices.

(c) Show that these selection rules hold independent of what atoms are in the primitive unit cell, so long as the lattice is bcc or fcc respectively.

All standard exam material

You should be able to do this all in your sleep.

(d) A collimated beam of monochromatic X-rays of wavelength 0.162 nm is incident upon a powdered sample of the cubic metal palladium. Peaks in the scattered X-ray pattern are observed at angles of 42.3°, 49.2°, 72.2°, 87.4° and 92.3° from the direction of the incident beam.

▷ Identify the lattice type

▷ Calculate the lattice constant and the nearest-neighbor distance.

▷ How well does this distance agree with the known data that the density of palladium is 12023 kg $\mathrm{m}^{-3}$? [Atomic mass of palladium = 106.4].

(e) How could you improve the precision with which the lattice constant is determined.

### 3.7. ‡ Neutron Scattering

(a) X-ray diffraction from sodium hydride (NaH) established that the Na atoms are arranged on a face-centred cubic lattice.

▷ Why is it difficult to locate the positions of the H atoms using X-rays?

All standard exam

The H atoms were thought to be displaced from the Na atoms either by $(\frac{1}{4}, \frac{1}{4}, \frac{1}{4})$ or by $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$, to form the ZnS (zinc blende) structure or NaCl (sodium chloride) structure, respectively. To distinguish these models a neutron powder diffraction measurement was performed. The intensity of the Bragg peak indexed as (111) was found to be much larger than the intensity of the peak indexed as (200).

▷ Write down expressions for the structure factors $S_{hkl}$ for neutron diffraction assuming NaH has

(i) the sodium chloride (NaCl) structure

(ii) the zinc blende (ZnS) structure.

▷ Hence, deduce which of the two structure models is correct for NaH. [Nuclear scattering length of Na = $0.363 \times 10^5$nm; nuclear scattering length of H = $-0.374 \times 10^5$ nm]

(b) How does one produce monochromatic neutrons for use in neutron diffraction experiments?

▷ What are the main differences between neutrons and X-rays?

▷ Explain why (inelastic) neutron scattering is appropriate for observing phonons, but x-rays are not.

### 3.8. One Dimensional Tight Binding Model

1d tight binding model has shown up on exams (albeit rarely)

Part (b) The diatomic case has never shown up though

This problem really belongs in problem set 2 due to its similarities with problems 2.5. and 2.6.. I recommend that you back up and review those problems before attempting this one. They are *extremely* similar to this.

(a) **Monatomic Solid:** Consider a one-dimensional tight binding model of electrons hopping between atoms. Let the distance between atoms be called $a$, and here let us label the atomic orbital on atom $n$ as $|n\rangle$ for $n = 1 \dots N$ (and you may assume periodic boundary conditions). Suppose there is an on-site energy $\epsilon$ and a hopping matrix element $-t$. In other words, suppose $\langle n|H|m\rangle = \epsilon$ for $n = m$ and $\langle n|H|m\rangle = -t$ for $n = m \pm 1$.

▷ Derive and sketch the dispersion curve for electrons. (Hint: Use the effective Schroedinger equations of problem 2.2.a. The resulting equation should look very similar to that of problem 2.5. above.)

Know the ideas of effective mass and density of states.

Also know when you have a metal vs insulator

▷ How many different eigenstates are there in this system?

▷ What is the effective mass of the electron near the bottom of this band?

▷ What is the density of states?

▷ If each atom is monovalent (it donates a single electron) what is the density of states at the fermi surface?

▷ What then is the Pauli paramagentic (spin) susceptibility of the system? (See problem 1.6.).

▷ What is the spin susceptibility if each atom is divalent?

(b) **Diatomic Solid:** Now consider a model of a diatomic solid as such

$$-A-B-A-B-A-B-$$

Suppose that the onsite energy of type $A$ is different from the onsite energy of type $B$. I.e, $\langle n|H|n\rangle$ is $\epsilon_A$ for $n$ being on a site of type $A$ and is $\epsilon_B$ for $n$ being on a site of type $B$. (All hopping matrix elements $-t$ are still identical to each other).

▷ Calculate the new dispersion relation. (This is extremely similar to problem 2.6. above. If you are stuck, try studying that problem again.)

▷ Sketch this dispersion relation in both the reduced and extended zone schemes.

▷ What happens in the "atomic" limit when $t$ becomes very small.

▷ What is the effective mass of an electron near the bottom of the lower band?

▷ If each atom (of either type) is monovalent, is the system a metal or an insulator?

This is very standard exam material too.

## Problem Set 4

### Band Structure and Semiconductor Physics

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### 4.1. Number of States in the Brillouin Zone

Worth knowing!

A specimen in the form of a cube of side L has a primitive cubic lattice whose mutually orthogonal fundamental translation vectors have length $a$. Show that the number of different allowed $\vec{k}$-states within the first Brillouin zone equals the number of primitive unit cells forming the specimen (do not consider spin). One may assume periodic boundary conditions, although it is worth thinking about whether this still holds for hard-wall boundary conditions as well.

### 4.2. ‡Nearly Free Electron Model

A question like this shows up every other year or so (maybe even more often)

Consider an electron in a weak periodic potential in one dimension $V(x) = V(x+a)$. Write the periodic potential as

$$V(x) = \sum_G e^{iGx} V_G$$

where the sum is over the reciprocal lattice $G = 2\pi n/a$, and $V_G^* = V_{-G}$ assures that the potential $V(x)$ is real.

You should be able to give both brief and more detailed answers depending on how it is asked.

(a) Explain why for $k$ near to a Brillouin zone boundary (such as $k$ near $\pi/a$) the electron wavefunction should be taken to be

$$\psi = Ae^{ikx} + Be^{i(k+G)x} \tag{1}$$

where $G$ is a reciprocal lattice vector such that $|k|$ is close to $|k+G|$.

Part c is rarely asked (or is considered difficult if it is asked)

(b) For an electron of mass $m$ with $k$ exactly at a zone boundary, use the above form of the wavefunction to show that the eigenenergies at this wavevector are

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

where $G$ is chosen so $|k| = |k+G|$.

Part d is worth knowing

▷ Give a qualitative explanation of why these two states are separated in energy by $2|V_G|$.

▷ Give a sketch (don't do a full calculation) of the energy as a function of $k$ in both the extended and the reduced zone schemes.

(c) *Now consider $k$ close to, but not exactly at, the zone boundary. Give an expression for the energy $E(k)$ correct to order $(\delta k)^2$ where $\delta k$ is the wavevector difference of $k$ to the zone boundary wavevector.

▷ Calculate the effective mass of an electron at this wavevector.

(d) Consider a two dimensional square lattice of divalent atoms. If the periodic potential is very very weak, you can consider the electrons to be free and to form a circular Fermi sea. Using the intuition from above (as well as the result of 4.1. above) sketch the Fermi surface for weak, medium, and strong periodic potentials.

▷ Roughly how strong should the periodic potential be for the system to be no longer a metal.

4.3. **Band Theory**

These are standard exam questions too

(a) Give a brief description of the formation of electron bands in crystals including reference to the atomic structure of the constituent atoms.

(b) Explain the following:

(i) sodium, which has 2 atoms in a bcc (conventional cubic) unit cell, is a metal;

(ii) calcium, which has 4 atoms in a fcc (conventional cubic) unit cell, is a metal;

(iii) diamond, which has 8 atoms in a fcc (conventional cubic) unit cell with a basis, is an electrical insulator, whereas silicon and germanium, which have similar structures, are semiconductors.

▷ Why is diamond transparent?

(c) A two-dimensional material has a square lattice with lattice constant $a$ =0.3 nm. The dispersion relations for electron energies in the conduction and valence bands are given by

$$\begin{aligned}\epsilon_c(\mathbf{k}) &= 6 - 2(\cos k_x a + \cos k_y a)\\ \epsilon_v(\mathbf{k}) &= -2 + (\cos k_x a + \cos k_y a)\end{aligned}$$

where energies are given here in units of eV. Sketch $\epsilon_c$ and $\epsilon_v$ for the direction $k_x = k_y$.

▷ Indicate the value and position of the minimum band gap.

▷ Show that close to the conduction and valence band edges, contours of constant energy are circles in $k$-space and..

▷ .. determine the effective masses of both the electrons and the holes.

▷ Sketch the density of states as a function of energy for the whole of both the conduction and the valence band.

(d) Using tight-binding theory, explain where the above dispersion relations come from.

4.4. **Law of Mass Action and Doping of Semiconductors**

Very standard exam question!

(a) Assume that the band gap energy $E_g$ is much greater than the temperature $k_bT$. Show that in a pure semiconductor at a fixed $T$, the product of the number of electrons ($n$) and the number of holes ($p$) depends only on the density of states in the conduction band and the density of states in the valence band (through their effective masses), and on the band gap energy.

▷ Derive expressions for $n$ for $p$ and for the product $np$. You may need to use the integral $\int_0^\infty dx x^{1/2} e^{-x} = \sqrt{\pi}/2$.

(b) The band gaps of Silicon and Germanium are 1.1 eV and 0.75 eV respectively. You may assume the effective masses for Silicon and Germanium are isotropic, roughly the same, and are roughly .5 of the bare electron mass for both electrons and holes. (Actually the effective masses are not quite the same, and furthermore the effective masses are both rather anisotropic.. but we are just making a rough estimates here).

▷ Estimate the conduction electron concentration for intrinsic (undoped) Silicon at room temperature.

▷ Make a rough estimate of the maximum concentration of ionized impurities that will still allow for this "intrinsic" behavior.

▷ Estimate the conduction electron concentration for Germanium at room temperature.

(c) The graph in Figure 1 shows the relationship between charge-carrier concentration for a certain n-doped semiconductor.

▷ Estimate the bandgap for the semiconductor and the concentration of donor ions.

▷ Describe in detail an experimental method by which this data could have been measured and suggest possible sources of experimental error.

Standard exam questions!

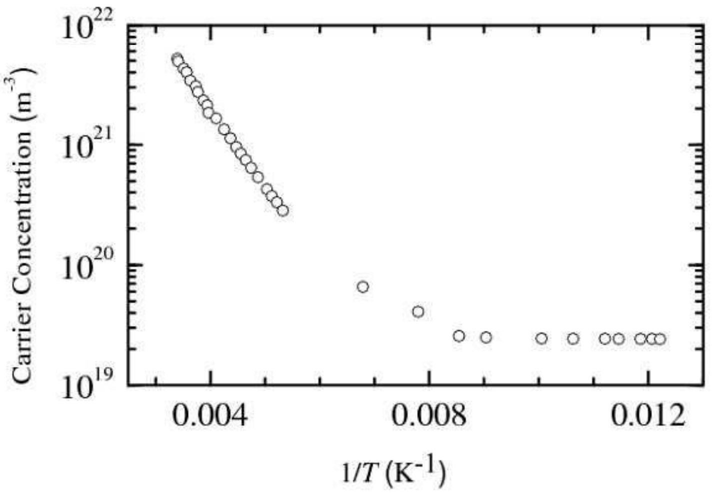


FIG. 1: Figure for Problem 4.4.

4.5. **More about Semiconductors**

(a) In semiconductor physics what is meant by a hole and why is it useful?

Know this (note the comments from revision lecture about signs!)

(b) An electron near the top of the valence band in a semiconductor has energy

$$E = -10^{-37}|\vec{k}|^2$$

where $E$ is in Joules and $k$ is in $\mathrm{m}^{-1}$. An electron is removed from a state $\vec{k} = 2 \times 10^8 \mathrm{m}^{-1}\hat{x}$ where $\hat{x}$ is the unit vector in the $x$-direction. For a hole, calculate (and give the sign of!)

(i) the effective mass

(ii) the energy

(iii) the momentum

(iv) the velocity.

(v) If there is a density $p = 10^5 \mathrm{m}^{-3}$ of such holes all having almost exactly this same momentum, calculate the current density and its sign.

(c)Show that the chemical potential in an intrinsic semiconductor lies in the middle of the gap at low temperature.

▷ Explain how the chemical potential varies with temperature if the semiconductor is doped with (i) donors (ii) acceptors.

This is standard too

(d) A direct gap semiconductor is doped to produce a density of $10^{23}$ electrons/m$^3$. Calculate the hole density at room temperature given that the gap is 1.0 eV, and the effective mass of carriers in the conduction and valence band are 0.25 and 0.4 electron masses respectively. Hint: use the result of problem 4.4..a.

### 4.6. **Semiconductor Quantum Well**

(a) A quantum well is formed from a layer of GaAs of thickness $L$ nm, surrounded by layers of $\mathrm{Ga}_{1-x}\mathrm{Al}_x\mathrm{As}$. You may assume that the band gap of the $\mathrm{Ga}_{1-x}\mathrm{Al}_x\mathrm{As}$ is substantially larger than that of GaAs. (The electron (hole) effective mass in GaAs is 0.068 $\mathrm{m_e}$ (0.45 $\mathrm{m_e}$) where $\mathrm{m_e}$ is the mass of the electron.)

▷ Sketch the shape of the potential for the electrons and holes.

▷ What approximate value of $L$ is required if the band gap of the quantum well is to be 0.1 eV larger than that of GaAs bulk material?

(b) *What might this structure be useful for?

▷ How would it be possible to n-dope this structure so that electrons accumulate in the well region of the structure, but away from impurities.

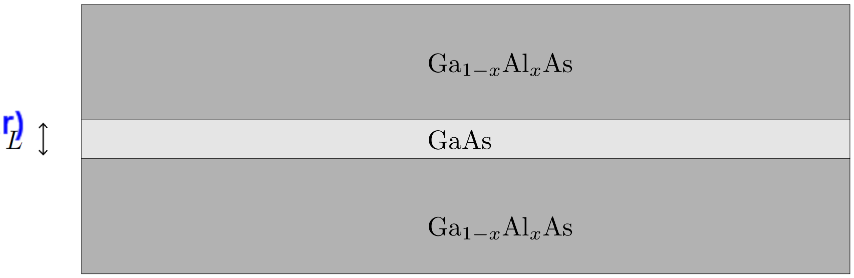
▷ Why would this be useful?

This used to be a standard exam question.

I think it is still examinable, but I'm wondering whether it is likely to show up, being that device physics has been de-emphasized

(it will be made nonexaminable next year)

It isn't hard so it is probably worth knowing just in case.



Magnetism in some form shows up frequently. But many aspects of magnetism are examined only rarely.

# Problem Set 5

## Magnetism and Mean Field Theory

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5.1. ‡ **General Magnetism**

part a you should know!

(a) Explain qualitatively why some atoms are paramagnetic and others are diamagnetic with reference to the electronic structure of these materials.

(b) Use Hund's rules and the Aufbau principle to determine $L$, $S$, and $J$ for the following isolated atoms:

Hund's rule is not examinable

(i) Sulfer (S) atomic number = 16

(ii) Vanadium (V), atomic number = 23

(iii) Zirconium (Zr), atomic number = 40

Worth knowing these definitions

(c) Define the terms Ferromagnetism, Antiferromagnetism, Ferrimagnetism, and Itinerant Ferromagnetism.

▷ Write down an example of a Hamiltonian which would have each one of these as its ground state.

Larmor diamag has shown up on exams.

(d) The wavefunction of an electron bound to an impurity in n-type silicon is hydrogenic in form. Estimate the impurity contribution to the diamagnetic susceptibility of a Si crystal containing $10^{20}\ m^{-3}$ donors given that the electron effective mass $m* = 0.4 m_e$ and the relative permitivity is $\epsilon_r = 12$.

▷ Make sure you know the derivation of the formula you use!

5.2. ‡ **Weiss Mean Field Theory of the Ferromagnet** Consider the spin-1/2, ferromagnetic Heisenberg Hamiltonian on the cubic lattice

This is probably the most common magnetism question!

$$\mathcal{H} = -\frac{J}{2}\sum_{<i,j>} \mathbf{S_i}\cdot\mathbf{S_j} + g\mu_B \mathbf{B}\sum_i \mathbf{S_i} \tag{1}$$

Here, $J > 0$, with the sum indicated with $< i, j >$ means summing over $i$ and $j$ being neighboring sites of the cubic lattice, and $\mathbf{B}$ is the externally applied magnetic field, which we will assume is in the $\hat{z}$ direction for simplicity. The factor of 1/2 out front is included so that each pair of spins is counted only once. Each site $i$ is assumed to have a spin $\mathbf{S_i}$ of spin $S = 1/2$. Here $\mu_B$ is the conventional Bohr magneton defined to be positive. The fact that the final term has a + sign out front is from the fact that the electron charge is negative, therefore the magnetic moment opposes the spin direction. If one were to assume that these were nuclear spins the sign would be reversed (and the magnitude would be much smaller due to the larger nuclear mass).

(a) Focus your attention on one particular spin $\mathbf{S_i}$, and write down an effective Hamiltonian for this spin, treating all other variables $\mathbf{S_j}$ with $j \neq i$ as expectations $\langle \mathbf{S_j} \rangle$ rather than operators.

(b) Calculate $\langle \mathbf{S_i} \rangle$ in terms of the temperature and the fixed variables $\langle \mathbf{S_j} \rangle$ to obtain a mean-field self-consistency equation.

▷ Write the magnetization $M = |\mathbf{M}|$ in terms of $\langle \mathbf{S} \rangle$ and the density of spins.

(c) At high temperature, find the susceptibility $\chi = dM/dH = \mu_0 dM/dB$ in this approximation.

(d) Find the critical temperature in this approximation.

▷ Write the susceptibility in terms of this critical temperature.

(e) Show graphically that in zero external field ($\mathbf{B} = 0$), below the critical temperature, there are solutions of the self consistency equation with $M \neq 0$.

(f) Repeat parts (a)-(d) but now assuming there is an $S = 1$ spin on each site (meaning that $S_z$ takes the values $-1, 0, +1$).

### 5.3. Bragg-Williams Approximation

Bragg-Williams has never been on an exam.

This problem provides a different approach to obtaining the Weiss mean-field equations. For simplicity we will again assume spin 1/2 variables on each site.

Assume there are $N$ lattice sites in the system. Let the average spin value be $\langle S_i \rangle = s$. Thus the probability the probability of a spin being an up spin is $P_\uparrow = 1/2 + s$ whereas the probability of any spin being a down spin is $P_\downarrow = 1/2 - s$. The total number of up spins or down spins is then $NP_\uparrow$ and $NP_\downarrow$ respectively where there are $N$ total lattice sites in the system.

(a) Consider first a case where sites do not interact with each other. In the micro-canonical ensemble, we can count the number of configurations (microstates) which have the given number of spin ups and spin downs (determined by $s$). Using $S = k_b \ln \Omega$ calculate the entropy of the system in the large $N$ limit.

(b) Assuming all sites have independent probabilities $P_\uparrow$ and $P_\downarrow$ of pointing up and down respectively, calculate the probability that two neighboring sites will point in the same direction and the probability that two neighboring sites will point in opposite directions.

▷ Use this result to calculate an approximation to the expectation of the Hamiltonian. Note: This is not an exact result, as in reality, sites that are next to each other will have a tendency to have the same spin because that will lower their energies, but we have ignored this effect here.

(c) Putting together the results of (a) and (b) above, derive the approximation to the free energy

$$F = E - TS = Nk_bT\left[(\frac{1}{2}+s)\log(\frac{1}{2}+s) + (\frac{1}{2}-s)\log(\frac{1}{2}-s)\right] + g\mu_B B_z N s - JNZs^2/2$$

where $Z$ is the number of neighbors each spin has, and we have assumed the external field to be in the $\hat{z}$ direction. (Again we assume the spin is electron spin so that the the energy of a spin interacting with the external field is $+g\mu_b \vec{B}\cdot\vec{S}$.)

(d) Extremize this expression with respect to the variable $s$ to obtain the same mean field equations as above.

▷ Below the critical temperature note that there are three solutions of the mean field equations.

▷ By examining the second derivative of $F$ with respect to $s$, show that the $s = 0$ solution is actually a maximum of the free energy rather than a minimum.

▷ Sketch $F(s)$ both above and below the critical temperature for $B = 0$. At nonzero $B$?

### 5.4. Mean Field Theory for the Antiferromagnet

Mean field theory for the antiferro has been on exams!

For this exercise we use the Molecular Field (Weiss Mean Field) approximation for the spin-1/2 *Antiferromagnetic* model on a 3 dimensional cubic lattice. The full Hamiltonian is exactly that of Eq. 1 above, except that now we have $J < 0$, so neighboring spins want to point in opposite directions. (Compared to a Ferromagnet where $J > 0$ and neighboring spins want to point in the same direction). For simplicity let us assume that the external field points in the $\hat{z}$ direction.

At mean field level, the ordered ground state of this Hamiltonian will have alternating spins pointing up and down respectively. Let us call the sublattices of alternating sites, sublattice $A$ and sublattice $B$ respectively (i.e, $A$ sites have lattice coordinates $(i,j,k)$ with $i+j+k$ odd whereas $B$ sites have lattice coordinates with $i+j+k$ even).

In Mean field theory the interaction between neighboring spins is replaced by an interaction with an average spin. Let $s_A = \langle S^z \rangle_A$ be the average value of the spins on sub-lattice $A$, and $s_B = \langle S^z \rangle_B$ be the average value of the spins on sub-lattice $B$. (We assume that these are also oriented in the $\pm\hat{z}$ direction).

(a) Write the mean field Hamiltonian for a single site on sublattice $A$ and the mean field Hamiltonian for a single site on sublattice $B$.

(b) Derive the mean-field self consistency equations

$$\begin{aligned} s_A &= \frac{1}{2}\tanh(\beta[JZs_B - g\mu_B B]/2) \\ s_B &= \frac{1}{2}\tanh(\beta[JZs_A - g\mu_B B]/2) \end{aligned}$$

with $\beta = 1/(k_b T)$. Recall that $J < 0$.

(c) Let $B = 0$. Reduce the two self-consistency equations to a single self consistency equation. (Hint: Use symmetry to simplify! Try plotting $s_A$ versus $s_B$).

(d) Assume $s_{A,B}$ are small near the critical point and expand the self consistency equations. Derive the critical temperature $T_c$ below which the system is antiferromagnetic (i.e., $s_{A,B}$ become nonzero).

(e) How does one detect antiferromagnetism experimentally?

(f) In this mean-field approximation, the magnetic susceptibility can be written as

$$\chi = -(N/2)g\mu_0\mu_B \lim_{B\to 0} \frac{\partial(s_A + s_B)}{\partial B}$$

(why the factor of 1/2 out front?).

▷ Derive this susceptibility for $T > T_c$ and write it in terms of $T_c$.

▷ Compare your result with the analogous result for a ferromagnet. (Problem 5.2.). In fact, it was this type of measurement that first suggested the existence of antiferromagnets!

**Part g would be way too hard for an exam I should think!**

(g)* For $T < T_c$ show that

$$\chi = \frac{(N/4)\mu_0(g\mu_b)^2(1-(2s)^2)}{k_b T + k_b T_c(1-(2s)^2)}$$

with $s$ the staggered moment (ie, $s(T) = |s_A(T)| = |s_B(T)|$).

▷ Compare this low $T$ result with that of part f.

▷ Give a sketch of the susceptibility at all $T$.

### 5.5. Ground States and Spin Waves

(a) Consider the spin-1 Heisenberg Hamiltonian from Problem 5.2.. Let us take $\mathbf{B}$ to be in the $-\hat{z}$ direction, and assume a cubic lattice.

It will be useful to remember that

$$\mathbf{S_i}\cdot\mathbf{S_j} = \frac{1}{2}(S_i^+ S_j^- + S_i^- S_j^+) + S_i^z S_j^z$$

(a.i) For $J > 0$, i.e., for the case of a ferromagnet, intuition tells us that the ground state of this Hamiltonian should simply have all spins aligned. Consider such a state. Show that this is an eigenstate of the Hamiltonian Eq. 1 and find its energy.

(a.ii) For $J < 0$, the case of an antiferromagnet, one might expect that, at least for $\mathbf{B} = 0$ the state where spins on alternating sites point in opposite directions might be an eigenstate. Unfortunately, this is not precisely true. Consider such a state of the system.

▷ Show that the state in question is not an eigenstate of the Hamiltonian.

Although the intuition of alternating spins on alternating sites is not perfect, it becomes reasonable for systems with large spins $S$. For smaller spins (like spin 1/2) one needs to consider these so-called "quantum fluctuations". (We will not do that here).

**It is not clear that spin waves are examinable in this paper. (They are clearly examinable in the 4th year option which makes it rather unlikely that they would be examined in the 3rd year exam)**

(b) For the spin-$S$ ferromagnet particularly for large $S$, our "classical" intuition is fairly good and we can use simple approximations to examine the excitation spectrum above the ground state.

First recall the Heisenberg equations of motion for any operator

$$i\hbar \frac{d\hat{O}}{dt} = [\hat{O}, \mathcal{H}]$$

with $\mathcal{H}$ the Hamiltonian (Eq. 1 with $\mathbf{S_i}$ being a spin $S$ operator).

(b.i) Derive equations of motion for the spins in the Hamiltonian Eq. 1. Show that one obtains

$$\hbar \frac{d\mathbf{S_i}}{dt} = \mathbf{S_i} \times \left( J \sum_j \mathbf{S_j} - g\mu_b \mathbf{B} \right) \tag{2}$$

where the sum is over sites $j$ that neighbor $i$.

(b.ii) In the ferromagnetic case, particularly if $S$ is large, we can treat the spins as not being operators, but rather as being classical variables. In the ground state, we can set all $\mathbf{S_i} = \hat{z}S$ (Assuming $\mathbf{B}$ is in the $-\hat{z}$ direction so the ground state has spins aligned in the $\hat{z}$ direction). Then to consider excited states, we can perturb around this solution by writing

$$\begin{aligned} S_i^z &= S - \mathcal{O}((\delta S)^2/S) \\ S_i^x &= \delta S_i^x \\ S_i^y &= \delta S_i^y \end{aligned}$$

where we can assume $\delta S^x$ and $\delta S^y$ are small compared to $S$. Expand the equations of motion (Eq. 2) for small perturbation to obtain equations of motion that are linear in $\delta S_x$ and $\delta S_y$

(b.iii) Further assume wavelike solutions

$$\begin{aligned} \delta S_i^x &= A_x e^{i\omega t - i\mathbf{k}\cdot\mathbf{r}} \\ \delta S_i^y &= A_y e^{i\omega t - i\mathbf{k}\cdot\mathbf{r}} \end{aligned}$$

This ansatz should look very familiar from our prior consideration of phonons.

Plug this form into your derived equations of motion.

▷ Show that $S_i^x$ and $S_i^y$ are out of phase by $\pi/2$. What does this mean?

▷ Show that the dispersion curve for "spin-waves" of a ferromagnet is given by $\hbar\omega = |F(\mathbf{k})|$ where

$$F(\mathbf{k}) = JS(6 - 2[\cos(k_x a) + \cos(k_y a) + \cos(k_z a)]) + g\mu_b |B|$$

where we assume a cubic lattice.

▷ How might these spin waves be detected in an experiment?

### 5.6. Itinerant Ferromagnetism

This has never been examined before, but it is now officially added to the syllabus.

I'd be a bit surprised if it showed up on the exam, but I suppose it could.

(a.i) Review 1: For a three dimensional tight binding model on a cubic lattice, calculate the effective mass in terms of the hopping matrix element $t$ between nearest neighbors and the lattice constant $a$.

(a.ii) Review 2: Assuming the density $n$ of electrons in this tight binding band is very low, one can view the electrons as being free electrons with this effective mass $m^*$. For a system of spinless electrons show that the total energy per unit volume (at zero temperature) is given by

$$E/V = nE_{min} + Cn^{5/3}$$

where $E_{min}$ is the energy of the bottom of the band.

▷ Calculate the constant $C$.

(b) Let the density of spin-up electrons be $n_\uparrow$ and the density of spin-down electrons be $n_\downarrow$ we can write these as

$$\begin{aligned} n_\uparrow &= (n/2)(1+\alpha) \qquad (3) \\ n_\downarrow &= (n/2)(1-\alpha) \qquad (4) \end{aligned}$$

where the total net magnetization of the system is given by

$$M = -\mu_b n \alpha$$

Using the result of part (a), fixing the total density of electrons in the system $n$,

▷ calculate the total energy of the system per unit volume as a function of $\alpha$.

▷ Expand your result to fourth order in $\alpha$.

▷ Show that $\alpha = 0$ gives the lowest possible energy.

▷ Argue that this remains true to all orders in $\alpha$

(c) Now consider adding a Hubbard interaction term

$$H_{hubbard} = U \sum_i N^i_\uparrow N^i_\downarrow$$

with $U \geq 0$ where $N^i_\sigma$ is the number of electrons of spin $\sigma$ on site $i$.

Calculate the expectation value of this interaction term given that the up and down electrons form fermi seas with densities $n_\uparrow$ and $n_\downarrow$ as given by Eqns. 3 and 4 above.

▷ Write this energy in terms of $\alpha$.

(d) Adding together the kinetic energy calculated in part b with the interaction energy calculated in part c, determine the value of $U$ for which it is favorable for $\alpha$ to become nonzero.

▷ For values of $U$ not too much bigger than this value, calculate the magnetization as a function of $U$.

▷ Explain why this calculation is only an approximation.

(e) Consider now a two dimensional tight binding model on a square lattice with a Hubbard interaction. How does this alter the result of part (d)?

Similar comment about Hubbard model In principle examinable, in practice unlikely.

### 5.7. Antiferromagnetism in the Hubbard Model

Consider a tight binding model with hopping $t$ and a strong Hubbard interaction.

$$H_{hubbard} = U \sum_i N_\uparrow^i N_\downarrow^i$$

(a) If there is one electron per site, if the interaction term $U$ is very strong, explain qualitatively why the system must be an insulator.

(b) On a square lattice, with one electron per site, and large $U$, use second order perturbation theory to determine the energy difference between the ferromagnetic state and the antiferromagnetic state. Which one is lower energy?

## Some Revision Problems

### 6.1. Debye Theory

Know this

Use the Debye approximation to determine the specific heat of a two dimensional solid as a function of temperature. State your assumptions. You will need to leave your answer in terms of an integral that generally one cannot do. At high $T$, show the specific heat goes to a constant and find that constant. At low $T$, show that $C_v = KT^n$ Find $n$. Find $K$ in terms of a definite integral. If you are brave you can try to evaluate the integral, but you will need to leave your result in terms of the Riemann zeta function $\zeta(s) = \sum_{n=1}^{\infty} n^{-s}$.

### 6.2. Debye Theory II

Could be asked I suppose

Physicists should be good at making educated guesses: Guess the element with the highest Debye temperature. The lowest? You might not guess the ones with the absolutely highest or lowest temperatures, but you should be able to get close.

### 6.3. Free Electron Theory

a,b,c should be easy. (d) would be too hard for an exam

(a) Explain what is meant by the Fermi energy, Fermi temperature and the Fermi surface of a metal.

(b) Show that the kinetic energy of a free electron gas in 3D is $(3/5)NE_F$ where $E_F$ is the fermi energy.

(c) Consider a two dimensional electron gas. Derive an expression for the density of states.

(d) *Calculate the specific heat at low temperature of this two dimensional electron gas. The following integral may be useful:

$$\int_{-\infty}^{\infty} dx \frac{x^2 e^x}{(e^x+1)^2} = \frac{\pi^2}{3}$$

### 6.4. Vibrations I

This would be a good exam question

(a) Consider a 1 dimensional mass and spring model of a crystal. Write down the dispersion curve $\omega(k)$ for this model (this should be easy by this time). Now write an expression for the specific heat of this 1 dimensional chain. You will inevitably have an integral that you cannot do.

(b)* However, you can expand exponentials for high temperature to obtain a high temperature approximation. It should be obvious that the high temperature limit should give heat capacity $C = k_B$ per atom (the law of Dulong-Petit in one dimension). By expanding to next nontrivial order, show that

$$C/N = k_B(1 - A/T^2 + \ldots)$$

where

$$A = \frac{\hbar^2 k}{6m}$$

where $m$ is the atomic mass and $k$ is the spring constant.

6.5. **Vibrations II** Consider a 1 dimensional spring and mass model of a crystal. Generalize this model to include springs not only between neighbors but also between second nearest neighbors. Let the spring constant between neighbors be called $\kappa_1$ and the spring constant between second neighbors be called $\kappa_2$. Let the mass of each atom be $M$.

This would be a good exam question too

(a) Calculate the dispersion curve $\omega(k)$ for this model.

(b) Determine the sound wave velocity, Show the group velocity vanishes at the Brillouin zone boundary.

6.6. **Reciprocal Lattice**

Know this!

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?

Consider now an orthorhombic face-centered lattice with conventional lattice constants $a_1, a_2, a_3$. What it the reciprocal lattice now?

6.7. **Scattering**

Know this

The Bragg angles of a certain reflection off of copper Is 47.75° at 20°C but is 46.60° at 1000°C. What is the coefficient of linear expansion of copper? (Note: the Bragg angle $\theta$ is half of the measured diffraction (deflection) angle $2\theta$).

6.8. **More scattering**

Know this!

KCl and KBr are alkali-halides with the same crystal structure as NaCl: fcc cubic with Na at (0,0,0) and Cl at (1/2,1/2,1/2). KBr shows X-ray diffraction peaks from planes (111) (200) (220) (331) (222) (400)(331)(420), but KCl shows peaks only at (200)(220)(222)(400)(420). Why might this be true?

6.9. **Semiconductors**

Know this too!

Describe experiments to determine the following properties of a semiconductor sample: (i) sign of the majority carrier, (ii) carrier concentration (assume that one carrier type is dominant), (iii) band gap, (iv) effective mass (v) mobility of the majority carrier.

6.10. **More Semiconductors**

same...

Outline the absorption properties of a semiconductor and how these are related to the band gap. Explain the significance of the distinction between a direct and an indirect semiconductor. What region of the optical spectrum would be being studied for a typical semiconducting crystal?

6.11. **Yet More Semiconductors**

same

Outline a model with which you could estimate the energy of electron states introduced by donor atoms into an n-type semiconductor. Write down an expression for this energy, explaining why the energy levels are very close to the conduction band edge.

6.12. **Magnetism**

Explain briefly the origin of diamagnetism and paramagnetism in atoms.

Yes, same

Consider a crystal of volume $V$ composed of $N$ identical atoms. Each atom has spin 1/2 and $g = 2$. Assume neighboring atoms do not interact, derive an expression for the paramagnetic susceptibility as a function of temperature in the high temperature limit. Explain how this system might be used to make a refrigerator. In reality what limits how well this works?

Discuss what is meant by "quenching" of orbital angular momentum and its consequences for paramagnetism.

Quenching would not be asked I think.

### 6.13. **Mean field theory**

This was an exam question

(a) $\beta$-Brass is an alloy containing equal numbers of of Cu and Zn atoms. Above a temperature of 730K, the atoms are arranged randomly on a body centered cubic lattice. Below 730K, the lattice becomes simple cubic with Cu atoms largely on the (0,0,0) position and the Zn atoms largely at the (1/2,1/2,1/2) position in the unit cell. The energy of the crystal depends on the occupancy of the sites and is given by

$$E = \frac{1}{2}\sum_{i,j} J\sigma_i\sigma_j$$

where $\sigma_i = +1$ if the site is occupied by a Cu atom and $\sigma_i = -1$ if the site is occupied by a Zn atom. Here the sum is restricted to nearest neighbors. Using mean field approximation show that

$$\langle|\sigma|\rangle = \tanh(zJ\langle|\sigma|\rangle)$$

what is $z$ ? (b) Estimate the magnitude of $J$ (c) Explain, in detail, how this ordering could be observed.

# Additional Problems

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## More problems associated with Problem Set 1

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### A.1.1. **Diatomic Einstein Solid***

Too hard

Having studied problem 1.1., consider now a solid made up of diatomic molecules. We can (very crudely) model this as a two particles in three dimensions, connected to each other with a spring, both in the bottom of a harmonic well.

$$H = \frac{\mathbf{p_1}^2}{2m_1} + \frac{\mathbf{p_2}^2}{2m_2} + \frac{k}{2}\mathbf{x_1}^2 + \frac{k}{2}\mathbf{x_2}^2 + \frac{K}{2}(\mathbf{x_1} - \mathbf{x_2})^2$$

Here $k$ is the spring constant holding both particles in the bottom of the well, and $K$ is the spring constant holding the two particles together. Assume that the two particles are distinguishable atoms.

(a) Analogous to problem 1.1. above, calculate the classical partition function and show that the heat capacity is again $3k_B$ per particle (i.e., $6k_B$ total).

(b)Analogous to problem 1.1. above, calculate the quantum partition function and find an expression for the heat capacity. Sketch the heat capacity as a function of temperature if $K \gg k$.

(c)** How does the result change if the atoms are indistinguishable?

For this problem you may find it useful to transform to relative and center-of-mass coordinates. If you find this difficult, for simplicity you may assume that $m_1 = m_2$.

### A.1.2. **Another review of free electron theory**

What is the *free electron model* of a metal. Define *Fermi energy* and *Fermi temperature*.

Why do metals held at room temperature feel cold to the touch even though their Fermi temperatures are much higher than room temperature?

This was an
exam question

A $d$-dimensional sample with volume $L^d$ contains $N$ electrons and can be described as a free electron model. Show that the Fermi energy is given by

$$E_F = \frac{\hbar^2}{2mL^2}(N a_d)^{2/d}$$

Find the numerical values of $a_d$ for $d = 1, 2$, and 3.

Show also that the density of states at the Fermi energy is given by

$$g(E_F) = \frac{Nd}{2L^d E_F}$$

Assuming the free electron model is applicable, estimate the Fermi energy and Fermi temperature of the following materials:

(a) Copper, a monovalent metal (with face-centered-cubic structure) having four atoms per unit cell, where the side of a unit cell has length 0.361 nm.

(b) A one dimensional organic conductor which has unit cell of length 0.8 nm, where each unit cell contributes one mobile electron.

### A.1.3. Heat Capacity of a Free Electron Gas**

Too hard

In problem 1.6..a we approximated the heat capacity of a free electron gas (in 3d). Calculate an exact expression for the specific heat of a metal at low temperature. Caution, be careful to account for the fact that the chemical potential is a function of temperature. Note: you will run into some nasty integrals. If you cannot evaluate these integrals you can rewrite them as series whose summation is known.

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More problems associated with Problem Set 2

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### A.2.1. LCAO Done Right

(a) In problem 2.2. we introduced the method of linear combination of Atomic orbitals. In that problem we assumed that our basis of orbitals is orthonormal. In this problem we will relax this assumption.

Too hard

Consider now many orbitals on each atom (and potentially many atoms). Let us write

$$|\psi\rangle = \sum_{i=1}^{N} \phi_i |i\rangle$$

for an arbitrary number $N$ of orbitals. Let us write the $N$ by $N$ overlap matrix $\mathcal{S}$ whose elements are

$$\mathcal{S}_{i,j} = \langle i|j\rangle$$

In this case do NOT assume that $\mathcal{S}$ is diagonal.

Using a similar method as in problem 2.2., derive the new “Schroedinger equation”

$$\mathcal{H}\boldsymbol{\phi} = E\mathcal{S}\boldsymbol{\phi} \tag{1}$$

With the same notation for $\mathcal{H}$ and $\phi$ as in problem 2.2.. This equation is known as a “generalized eigenvalue problem” because of the $\mathcal{S}$ on the right hand side.

(b)** Let us now return to the situation with only two atoms and only one orbital on each atom but such that $\langle 1|2\rangle = \mathcal{S}_{1,2} \neq 0$. Without loss of generality we may assume $\langle i|i\rangle = 1$ and $S_{1,2}$ is real. If the atomic orbitals are $s$-orbitals then we may assume also that $t$ is real and positive (why?).

Use the above Eq. 1 to derive the eigenenergies of the system. Argue again the the energy gained in the bonding orbital is sufficient to overcome the repulsion between nuclei.

### A.2.2. LCAO and the Ionic-Covalent Crossover

unlikely
(see above
comments on
bonding)

(a) For problem 2.2..b consider now the case where the atomic orbitals $|1\rangle$ and $|2\rangle$ have unequal energies $\epsilon_{0,1}$ and $\epsilon_{0,2}$. As the difference in these two energies increases show that the bonding orbital becomes more localized on the lower energy atom. (For simplicity you may use the orthogonality assumption $\langle 1|2\rangle = 0$). Explain how this calculation can be used to describe a crossover between covalent and ionic bonding.

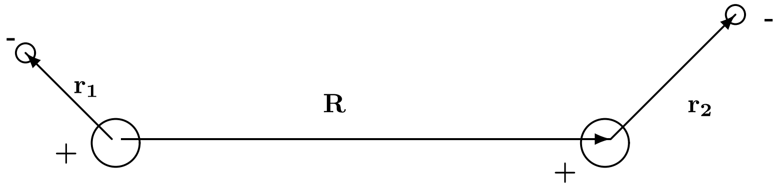
### A.2.3. Van der Waals Bonding in Detail*

Way too hard

(a) *Here we will do a much more precise calculation of the van der Waals force between two hydrogen atoms. First, let the position of the two nuclei be separated by a vector $\mathbf{R}$ as shown in the figure. Let us write the Hamiltonian for both atoms (assuming fixed positions of nuclei) as

$$\begin{aligned} H &= H_0 + H_1 \\ H_0 &= \frac{\mathbf{p_1}^2}{2m} + \frac{\mathbf{p_2}^2}{2m} - \frac{e^2}{4\pi\epsilon_0|\mathbf{r_1}|} - \frac{e^2}{4\pi\epsilon_0|\vec{r}_2|} \\ H_1 &= \frac{e^2}{4\pi\epsilon_0|\mathbf{R}|} + \frac{e^2}{4\pi\epsilon_0|\mathbf{R}+\mathbf{r_1}+\mathbf{r_2}|} - \frac{e^2}{4\pi\epsilon_0|\mathbf{R}+\mathbf{r_1}|} - \frac{e^2}{4\pi\epsilon_0|\mathbf{R}+\mathbf{r_2}|} \end{aligned}$$

as shown in the figure



Here $H_0$ is the Hamiltonian for two noninteracing hydrogen atoms, and $H_1$ is the interaction between the atoms.

Without loss of generality, let us assume that $\mathbf{R}$ is in the $\hat{x}$ direction. Show that for large $\vec{R}$ and small $\vec{r_i}$, the interaction Hamiltonian can be written as

$$H_1 = \frac{e^2}{4\pi\epsilon_0|\mathbf{R}|^3}(z_1z_2 + y_1y_2 - 2x_1x_2) + \mathcal{O}(1/R^4)$$

where $x_i, y_i, z_i$ are the components of $\mathbf{r_i}$. Show that this is just the interaction between two dipoles.

(b) **Perturbation Theory:** The eigenvalues of $H_0$ can be given as the eigenvalues of the two atoms separately. Recall that the eigenstates of hydrogen are written in the usual notation as $|n,l,m\rangle$ and have energies $E_n = -\text{Ry}/n^2$ with $\text{Ry} = me^4/(32\pi^2\epsilon_0^2\hbar^2) = e^2/(8\pi\epsilon_0 a_0)$ the Rydberg (Here $l \geq 0$, $|m| \leq l$ and $n \geq l+1$). Thus the eigenstates of $H_0$ are written as $|n_1, l_l, m_1; n_2, l_2, m_2\rangle$ with energies $E_{n_1,n_2} = -\text{Ry}(1/n_1^2 + 1/n_2^2)$. The ground state of $H_0$ is $|1,0,0;1,0,0\rangle$. Perturbing $H_0$ with the interaction $H_1$, show that to first order in $H_1$ there is no change in the ground state energy. Thus conclude that the leading correction to the energy ground state energy is proportional to $1/R^6$ (and hence the force is proportional to $1/R^7$). Recalling second order perturbation theory show that we have a correction to the total energy given by

$$\delta E = \sum_{n_1,n_2,l_1,l_2,m_1,m_2} \frac{|<1,0,0;1,0,0|\; H_1\; |n_1,l_l,m_1;n_2,l_2,m_2\rangle|^2}{E_{0,0} - E_{n_1,n_2}}$$

Show that the force must be attractive.

(c)* **Bounding the binding energy:** First, show that the numerator in this expression is zero if either $n_1 = 1$ or $n_2 = 1$. Thus the smallest $E_{n_1,n_2}$ that appears in the denominator is $E_{2,2}$. If we replace $E_{n_1,n_2}$ in the denominator with $E_{2,2}$ then the $|\delta E|$ we calculate will be greater than than the $|\delta E|$ in the exact calculation. On the other hand, if we replace $E_{n_1,n_2}$ by 0, then we the $|\delta E|$ will always be less than the $\delta E$ of the exact calculation. Make these replacements, and perform the remaining sum by identifying a complete set. Derive the bound

$$\frac{6e^2a_0^5}{4\pi\epsilon_0 R^6} \leq |\delta E| \leq \frac{8e^2a_0^5}{4\pi\epsilon_0 R^6}$$

You will need the matrix element for a hydrogen atom

$$\langle 1,0,0|x^2|1,0,0\rangle = a_0^2$$

where $a_0 = 4\pi\epsilon_0\hbar^2/(me^2)$ is the Bohr radius. (This last identity is easy to derive if you remember that the ground state wavefunction of a hydrogen atom is proportional to $e^{-r/2a_0}$ ).

Too hard

A.2.4. **General Proof That Normal Modes Become Quantum Eigenstates** This proof generalizes the argument given in problem 2.4.. Consider a set of $N$ particles $a = 1, \ldots N$ with masses $m_p$ interacting via a potential

$$U = \frac{1}{2}\sum_{a,b} x_a V_{a,b} x_b$$

where $x_a$ is the deviation of the position of particle $a$ from its equilibrium position and $V$ can be taken (without loss of generality) to be a symmetric matrix. (Here we consider a situation in 1d, however, we will see that to go to 3d we just need to keep track of 3 times as many coordinates).

(i) Defining $y_a = \sqrt{m_a}x_a$ show that the classical equations of motion may be written as

$$\ddot{y}_a = -\sum_b S_{a,b}\, y_b$$

where

$$S_{a,b} = \frac{1}{\sqrt{m_a}} V_{a,b} \frac{1}{\sqrt{m_b}}$$

Thus show that the solutions are

$$y_a^{(m)} = e^{-i\omega_m t} s_a^{(m)}$$

where $\omega_m$ is the $m^{th}$ eigenvalue of the matrix $S$ with corresponding eigenvector $s_a^{(m)}$. These are the $N$ normal modes of the system.

(ii) Recall the orthogonality relations for eigenvectors of hermitian matrices

$$\sum_a [s_a^{(m)}]^*[s_a^{(n)}] \;=\; \delta_{m,n} \tag{2}$$

$$\sum_m [s_a^{(m)}]^*[s_b^{(m)}] \;=\; \delta_{a,b} \tag{3}$$

Since $S$ is symmetric as well as hermitian, the eigenvectors can be taken to be real. Construct the transformed coordinates

$$Y^{(m)} \;=\; \sum_a s_a^{(m)} x_a \sqrt{m_a} \tag{4}$$

$$P^{(m)} \;=\; \sum_a s_a^{(m)} p_a / \sqrt{m_a} \tag{5}$$

show that these coordinates have canonical commutations

$$[P^{(m)}, Y^{(n)}] = -i\hbar\delta_{n,m} \tag{6}$$

and show that in terms of these new coordinates the Hamiltonian is rewritten as

$$H = \sum_m \left[ \frac{1}{2} [P^{(m)}]^2 + \frac{1}{2} \omega_m^2 [Y^{(m)}]^2 \right] \tag{7}$$

Conclude that the quantum eigenfrequencies of the system are also $\omega_m$. (Can you derive this result from the prior two equations?)

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More problems associated with Problem Set 3

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### A.3.1. And More X-ray scattering

A sample of Aluminum powder is put in an Debye-Scherrer X-ray diffraction device. The incident X-ray radiation is from Cu-Ka Xray transition (this just means that the wavelength is l = 1.54 Angstrom)

Know this

The following scattering angles were observed:

19.48° 22.64° 33.00° 39.68° 41.83° 50.35° 57.05° 59.42°

Given also that the atomic weight of Al is 27, and the density is 2.7 g/cm$^3$, use this information to calculate Avagadros number. How far off are you? What causes the error?

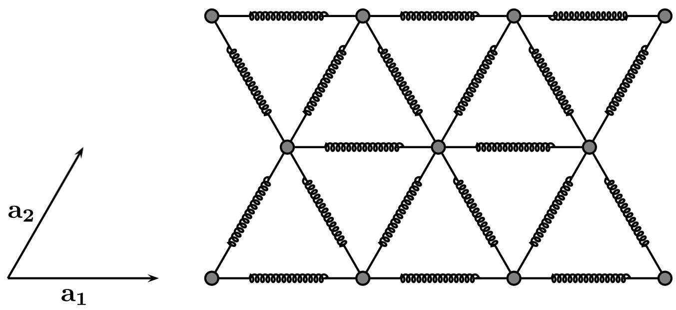
### A.3.2. Still More X-ray scattering

Know this

The unit cell dimension for a particular b.c.c. solid is 2.4 Angstrom. Two orders of diffraction are observed. What is the minimum Energy of the neutrons? At what T would such neutrons be dominant If the distribution is Maxwell Boltzmann.

### A.3.3. Phonons in 2d

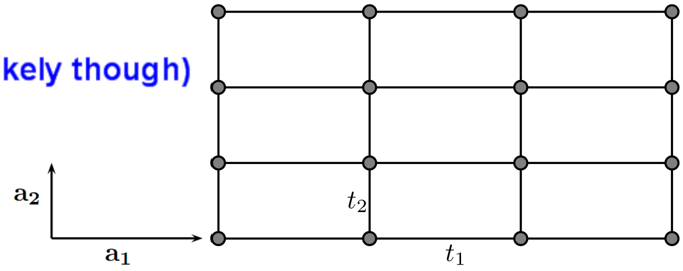
Too hard I think



Consider a mass and spring model of a two dimensional triangular lattice (assume the lattice is extended infinitely in all directions). Assume that each mass is attached to each of its 6 neighbors by equal springs of equal length. Find the first Brillouin zone. Calculate the dispersion curve $\omega(\mathbf{k})$.

### A.3.4. Tight Binding in 2d

Maybe? (unlikely though)



Consider a rectangular lattice in 2 dimensions with lattice constants $a_1$ in the horizontal direction and $a_2$ in the vertical direction. Describe the first Brillouin zone for this lattice.

Now imagine a tight binding model where there is one orbital at each lattice site, and where the hopping matrix element is $\langle n|H|m\rangle = t_1$ if sites $n$ and $m$ are neighbors in the horizontal direction and is $= t_2$ if $n$ and $m$ are neighbors in the vertical direction. Calculate the dispersion relation for this tight binding model. What does the dispersion relation look like near the bottom of the band?

### A.3.5. Diatomic Tight Binding Model: Peierls disortion

Consider a chain made up of all the same type of atom, but in such a way that the spacing between atoms alternated as long-short-long-short as follows

too hard I think

$$-A = A - A = A - A = A-$$

In a tight binding model, the shorter bonds (marked with $=$) will have hopping matrix element $t_{short} = t(1+\epsilon)$ whereas the longer bonds marked with $-$ have hopping matrix element $t_{long} = t(1-\epsilon)$. Calculate the tight-binding energy spectrum of this chain. (The onsite energy $\epsilon$ is the same on every atom). Expand your result to linear order in $\epsilon$. Suppose the lower band is filled and the upper band is empty (what is the valence of each atom in this case?). Calculate the total ground state energy of the filled lower band, and show it decreases linearly with increasing $\epsilon$.

Now consider a chain of equally spaced identical $A$ atoms connected together with identical springs with spring constant $\kappa$. Show that making a distortion whereby every other spacing is shorter by $\delta x$ costs energy proportional to $(\delta x)^2$. Conclude that for a chain with the valence discussed above, a distortion of this sort will occur spontaneously. This is known as a Peierls distortion.

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More problems associated with Problem Set 4

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### A.4.1. Hall resistivity with both electrons and holes

add this problem.

### A.4.2. p-n junction

[ Note: Presumably p-n junction is not supposed to be on the syllabus, but for years it was a standard question.]

Explain the origin of the depletion layer in an abrupt p-n junction and discuss how the junction causes rectifcation to occur. Stating your assumptions, show that the total width $w$ of the depletion layer of a p-n junction is:

$$w = w_n + w_p$$

**not examinable**

where

$$w_n = \left( \frac{2\epsilon_r \epsilon_0 N_A \phi_0}{e N_D (N_A + N_D)} \right)^{1/2}$$

and a similar expression for $w_p$ Here $\epsilon_r$ is the relative permittivity and $N_A$ and $N_D$ are the acceptor and donor densities per unit volume, while $\phi_0$ is the difference in potential across the p-n junction with no applied voltage. Calculate the total depletion charge and infer how this changes when an additional voltage, $V$ ,is applied.

What is the differential capacitance of the diode and why might it be useful to use a diode as a capacitor in an electronic circuit?

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## More problems associated with Problem Set 5

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### A.5.1. Spin $J$ Paramagnet

Given the hamiltonian for a system of noninteracting spin-$J$ atoms

**Likely to be too hard but possible**

$$\mathcal{H} = \tilde{g}\mu_B \mathbf{B} \cdot \mathbf{J}$$

Determine the magnetization as a function of $B$ and $T$. Show that the susceptibility is given by

$$\chi = \frac{\rho \mu_0 (\tilde{g}\mu_B)^2}{3} \frac{J(J+1)}{k_B T}$$

where $\rho$ is the density of spins.

### A.5.2. Correction to Mean Field

**Too hard**

Consider the spin-1/2 Ising Ferromagnet on a cubic lattice in $d$ dimensions. When we consider mean field theory, we treat exactly a single spin $\sigma_i$ and the $z = 2d$ neighbors on each side will be considered to have an average spin $\rightarrow \langle\sigma\rangle$. The critical temperature you calculate should be $k_b T_c = Jz/4$.

To improve on mean field theory, we can instead treat a block of two connected spins $\sigma_i$ and $\sigma_{i'}$ where the neighbors outside of this block are assumed to have the average spin $\rightarrow \langle\sigma\rangle$. Each of the spins in the block has $2d - 1$ such averaged neighbors. Use this improved mean field theory to write a new equation for the critical temperature (it will be a transcendental equation). Is this improved estimate of the critical temperature higher or lower than that calculated in the more simple mean-field model?