PHYS4450 Solid State Physics Problem Set 4 Due: 26 March 2013 (Tuesday)

All problem sets should be handed in not later than 5:00pm on the due date. Drop your assignment in the Box in Rm.213.

You should work out the steps of the calculations in detail.

4.0 *Reading Assignment:* Starting Chapter VIII, we deal with **electrons in solids**. Chapter VIII deals with the free electron model of metals, as discussed in Kittel's Chapter 6 and our Stat Mech course (ideal Fermi Gas). Chapters IX and XI discuss the effects of a periodic potential and thus energy band theory. Kittel's Chapter 7, plus part of Chapter 9 (on band structure calculations) and Secs. 7.1-7.4 and Secs. 8.3-8.4 of Christman's book are useful. Omar's Chapters 4 (free electron model) and 5 (band theory) give a clear explanation of the physics. For students who want a (very) serious treatment of band theory and its numerical implementations (usually for postgraduate students who need to do such work), the book *Electronic Structure: Basic Theory and Practical Methods* by R. Martin will be useful. Band structure calculations is a branch of research with never-ending possibilities, since new materials emerge all the time.

Problems 4.1 and 4.2 supplement the discussions on the Drude model. Problem 4.2 brings out the Drude formula for the dielectric constant of metals (AC frequencies). Problem 4.3 is on the empty lattice approximation.

4.1 **Drude model of conductivity – filling in some physics.** Either read pages VIII-43-46 or DIY here. When an electron of charge (-e) is acted upon by a static electric field, it should experience an acceleration. Thus, Newton's law would imply that the electron will move faster and faster in time. Current is the number of change passing through a point per unit time. **If** the charge carriers keep on moving faster and faster, one would expect that the current should keep on increasing with time after an electric field is switched on. This is obviously NOT our daily-life experience. When we wire up a circuit and connect it to a battery, the current reading in an ammeter will increase and then get at a steady value (no longer increasing with time). Thus, the electrons in a conductor do NOT accelerate after a while, i.e., the electrons instead attain a **terminal velocity** or a drift velocity $\mathbf{v}_D$. From Newtonian mechanics, there is an electric force and yet the electron attains a constant drift velocity, there must also be a frictional or damping force opposing the driving force (electric force). The electrons must suffer a lot of collisions. To model the effect of the collisions, a time τ called the collision time or relaxation time is introduced. Formally, the equation of motion for an electron becomes

$$\frac{d\mathbf{p}}{dt} = -e\mathbf{E} - \frac{\mathbf{p}}{\tau},$$

where $\mathbf{p}$ is the momentum, or

$$m\frac{d\mathbf{v}_D}{dt} = -e\mathbf{E} - \frac{m\mathbf{v}_D}{\tau}.$$

(a) Obtain the drift velocity in the steady state. Recall that "steady state" means there is no change with time and thus the $d\mathbf{p}/dt = m d\mathbf{v}_D/dt$ term vanishes (can be ignored) in the steady state. In physics literature, this step is expressed as "neglecting the inertial term" (an unnecessary fancy way to say something simple), where by "inertial" it means the term that goes with the mass. Thus, in the steady state, the damping term is important and the inertial term is not.

(b) In fact, one could solve the equation for $v_D(t)$ exactly. Try it out. Doing this gives us a reason why τ is called the relaxation time. In the form of $v_D(t)$, we will see how v_D increases from 0 to its steady state value after the electric field is switched on. Let's say we start with the steady state drift velocity. At some time called time zero again, switch OFF the field, and we know that eventually v_D will go back to zero. Show explicitly how v_D varies with time. Do you see that v_D relaxes back to its equilibrium value (zero) with τ being a characteristic time? [Notes: (i) Compare with the behavior in RC circuit. (ii) Collisions are important – they are responsible for maintaining a steady state at long time (where the effects of the field $\mathbf{E}$ is counterbalanced by the damping caused by collisions AND they are also responsible for helping a perturbed system (influenced by **E** at the beginning) get back to equilibrium. (iii) Think like a physicist – When there is a τ in the equations, **it sets a time scale**. Then it defines a boundary between **short time** and **long time**. For time $t \gg \tau$, we are in the long time limit and we have a steady state. For $t < \tau$, we are in the transient stage, where physical quantities vary with time. Carry this point with you when we consider AC case in Problem 4.2.

(c) The current density $\mathbf{J}$ is related to the electric field through $\mathbf{J} = \sigma\mathbf{E}$. But $\mathbf{J}$ is also related to the drift velocity of the carriers (electrons in a metal) by $\mathbf{J} = (-e)n\mathbf{v}_D$, where n is the number of (conduction) electrons per unit volume. Combining the relations, show that

$$\sigma = \frac{ne^2\tau}{m}, \tag{1}$$

which is a key equation in the transport properties of solids.

Remark: This is a typical phenomenological treatment in solid state physics. Up to now, we don't need to state clearly the origin(s) of the collisions (scatterings) that lead to τ. Much physics is hidden into an empirical parameter τ. In fact, Drude did not get the reason correctly (and don't blame him, he didn't know quantum mechanics), but the Drude formula remains valid and useful when we understand what τ means.

(d) **See SQ13. Getting some sense on numbers.** Take a metal (except sodium as it was done by TA in SQ13), e.g. gold (Au) or potassium (K). Consult the steps in SQ13. First, find the electron number density n. (There are many ways to do that, e.g. looking up the crystal structure and number of (conduction) electrons per atom, or using the mass density to obtain the lattice constant, etc.) Look up data for the conductivity or resistivity of Au (or K). Evaluate τ and $v_F\tau$. The latter quantity is called the mean free path.

Remark: We will see that the conductivity σ of a metal has to do with scattering of electrons due to **DEVIATIONS of the crystal from perfect periodicity**. The τ, besides carrying the meaning of relaxation time (as seen in part (b)), only carries the meaning of the mean time between successive collisions.

(e) Write down (no derivation needed) the **density of states per unit volume** for a free electron gas. Call it $g(E)$. Then start with the Drude formula for conductivity $\sigma = ne^2\tau/m$ and show that it can be re-written in the form

$$\sigma = \frac{ne^2\tau}{m} = \frac{1}{3}e^2 g(E_F) v_F^2 \tau,$$

where v_F is the Fermi velocity and $g(E_F)$ is the density of states per unit volume at the Fermi energy.

(f) **Mott argument.** Note that the combination $v_F\tau$ is the electron mean free path ℓ. Electron-phonon scattering is a main cause of resistance for metals at room temperature. In addition, electron-impurity scattering is another important source of resistance and it is always there (no temperature dependence).

Sir Nevill Mott (1905-1996) [1977 Nobel Physics Prize] noticed this point and argued that when more and more impurities are added to a metal, the mean free path will gradually be shortened and hence the conductivity decreases. Here enters the question whether a **dirty conductor** will eventually become an insulator and how. In Mott's view, the mean free path $v_F\tau$ drops, but it can only be as short as the lattice spacing a. Smaller than that, electrons cannot move away from the atom that they belong to and thus cannot take part in electrical conduction. Sounds reasonable, right? Mott said that there would be a *minimum* value of the conductivity as impurity concentration increases. Further increasing the impurity concentration will lead to *a sudden drop* of the conductivity to zero, i.e., a finite discontinuous jump. This is Mott's view of a **metal-insulator transition**. **Make an estimate of this minimum conductivity, using typical values of the parameters.**

A story as further remarks: There were physicists who argued that the transition from a metal to an insulator should be continuous (i.e., no finite jump). The physical argument is different and it has to do with a phenomenon called localization of electrons. Many experiments have been done to study the two proposals. Mott, Philip W. Anderson, and John Van Vleck were awarded the 1977 Nobel Prize for their contributions to the understanding of disordered systems (meaning solids but not in perfect order) and magnetism. Anderson was Van Vleck's PhD student at Harvard. Van Vleck was the first generation of physicists who applied quantum mechanics to understand valence, magnetism, and atomic and molecular spectrum. Anderson (age 89 now, in Princeton) is still a leading theorist. His contributions include the understanding of local moment formation of magnetic impurities in non-magnetic metals (Anderson model), Kondo problem, Josephson effect (Anderson was a visitor at Cambridge when Brian Josephson discovered the effect in superconductors under his name and Anderson was partly responsible for the discovery, but Josephson received the Nobel Prize alone for this effect), high T_c superconductors, etc. Collectively speaking, the most important contribution of Anderson to solid state physics is his idea of **spontaneous symmetry breaking** (related to 2008 Nobel Prize) in describing various physical phenomena in solids. His book *Basic Notions of Condensed Matter Physics* is a good place to learn about his many ideas. His recent book *The Theory of Superconductivity in the High-T_c Cuprates* contains his important and personal views on the unsolved problem of the origin of high-T_c superconductors. In 2011, he published a book *More is different* on his views on many different branches of science and other topics. Sir Mott also wrote many books. His early contributions were made in applying quantum mechanics to understand scattering of particles (e.g., electrons scattered off an atom). His books *Physics of Metals* and *Conduction in non-crystalline solids* are classics in solid state physics. His early textbook *Elements of Wave Mechanics* (published in 1950s) educated generations of physics students on quantum mechanics.

4.2 (**From DC to AC – Drude model of dielectric constants of metals and Optical Properties of Metals.**) This is an extension of the Drude model and it serves as an Appendix to Chapter VIII. [Put this at the end of Chapter VIII.] **(Together with SQ15 on the effect of both an electric and magnetic field, you have a complete set of notes on the Drude model.)**

We obtained $\sigma_0 = ne^2\tau/m$ for the conductivity for a conductor in response to a DC (static) applied field $\mathbf{E}$. Here, the subscript "0" labels the $\omega = 0$ static case. The question is whether the equation is still good for AC fields (i.e., oscillating field of angular frequency ω).

Let's think like a physicist! In our discussion of the formula, the characteristic time τ in the equation is the average time between consecutive collisions. In getting the formula, the idea is that collisions dominate the physics (many collisions that provide the damping term leading to the terminal drift velocity). Now for an AC field of finite frequency ω, **another time scale** corresponding to the period $\sim 1/\omega$ enters the problem. Thus, when there are **many collisions** in a period (slowly varying field), we expect that the physics is still dominated by collisions and hence $\sigma = ne^2\tau/m$ should still be good. Follow?

(a) Following this idea, show that the criterion that the static result remains valid for AC fields is $\omega\tau \ll 1$. [Note: A typical value of $\tau \approx 10^{-14}$ s (see number for your chosen metal). Thus, the DC formula actually works for a wide range of frequencies, e.g., from static to radio frequencies and all the way to about 10^{11} or even 10^{12} Hz. That's nice – a simple formula of static case works all the way to $\omega \ll 1/\tau$.]

(b) For frequencies higher than 10^{11} Hz or so, we need to be more careful. [See, we are even getting close to the optical range!] Let's start again with the equation

$$\frac{d\mathbf{p}}{dt} = -e\mathbf{E} - \frac{\mathbf{p}}{\tau}$$

and think like a physicist. Technically, the term on the left-hand side can be called the **inertial term** (recall it is ma as in $F = ma$), the two terms on the right-hand side can be called the **driving term** and the **damping term**, respectively. In the DC case, the physics comes from the competition between the driving and damping terms, i.e., the inertial term is not important in the DC case. Doing that, we obtain the terminal velocity and then σ_0.

Now let's keep all the terms and consider AC field. Like what you did in Mechanics (solving damped and forced oscillator problems) and in EM (handling Maxwell's equations), it is convenient to use a complex notation and assume harmonic time of the form $e^{-i\omega t}$ for the physical quantities. [The physical quantity is the real part of the complex counterpart. See Griffiths' EM textbook Sec.9.1 for a discussion, if needed. For engineers, they will take the form $e^{+j\omega t}$ instead and the results that follow will be slightly different in signs. But the physics is the same.] Therefore, we can write $\mathbf{p} = \mathbf{p}_0 e^{-i\omega t}$ and similar expressions for $\mathbf{E}$, $\mathbf{v}$ (velocity), and $\mathbf{J}$ (current density). Show that the amplitude $\mathbf{p}_0$ is given by

$$\mathbf{p}_0 = \frac{-e\mathbf{E}_0\tau}{1 - i\omega\tau}.$$

Here, the main point is that a term $i\omega\tau$ (and therefore ω) gets into the denominator.

(c) **AC Drude conductivity.** Expressing $\mathbf{p}$ in terms of of mass and velocity and then invoking the current density $\mathbf{J} = -en\mathbf{v}$, show that

$$\mathbf{J}_0 = \frac{\sigma_0}{1 - i\omega\tau}\mathbf{E}_0, \tag{2}$$

where $\sigma_0 = ne^2\tau/m$ is the static conductivity. Thus, you get a **frequency-dependent COMPLEX conductivity** at finite frequencies given by

$$\sigma(\omega) = \frac{\sigma_0}{1 - i\omega\tau}. \tag{3}$$

This is a **general result** for arbitrary ω (Drude model). In particular, for $\omega\tau \ll 1$, it gives the DC result (as discussed in part (a)).

(d) **Optical Properties of Metals.** Let's explore what is the meaning of a complex $\sigma(\omega)$. Is a complex conductivity real? [The latter "real" should be interpreted in English sense, not mathematical sense!] Here, we are stepping into the **optical properties of metals**. First, for whatever quantity, the **physical field** $\mathbf{A}_{phy} = Re[\mathbf{A}_0 e^{-i\omega t}]$, i.e., the real part of its complex counterpart. This works for $\mathbf{J}$, $\mathbf{E}$, etc. We have

$$\begin{aligned} \mathbf{J}_{phy} &= Re\left[\sigma(\omega)\mathbf{E}_0 e^{-i\omega t}\right] \\ &= Re\left[(\sigma_1(\omega) + i\sigma_2(\omega))\mathbf{E}_0 e^{-i\omega t}\right] \end{aligned} \tag{4}$$

where σ_1 and σ_2 are the real and imaginary parts of $\sigma(\omega)$.

Write down $\mathbf{E}_{phy}$ explicitly. Write down σ_1 and σ_2, and write down $\mathbf{J}_{phy}$ using the real part of the right hand side. Physics: Note that the physical response $\mathbf{J}_{phy}$ now carries both $\cos(\omega t)$ and $\sin(\omega t)$ terms, although the stimulation $\mathbf{E}_{phy}$ carries only $\cos(\omega t)$ term! [Recall: The phasor treatment in Year 1 physics (EM).] Look at σ_1 and σ_2. Physically, it says that at zero frequency and low frequencies, the current can follow the applied field very well, i.e., they are **in phase**. However, as frequency increases, the response (i.e., $\mathbf{J}_{phy}$) starts to have a part that is **out of phase** with the stimulation (i.e., the field). The total response $\mathbf{J}$ thus has a phase angle ϕ relative to the field. The larger (smaller) the imaginary part $\sigma_2(\omega)$ is, the larger (smaller) is the lag in phase characterized by ϕ. (Do you follow the physics?) That is to say, the complex $\sigma(\omega)$ is real stuff, it represents real physics!

(e) To further illustrate the physics. We know that heat is generated when we pass current through a conductor. From EM, it is represented by the **Joule heating** term $\mathbf{J} \cdot \mathbf{E}$. Of course, these fields are physical fields. Obtain $\mathbf{J}_{phy} \cdot \mathbf{E}_{phy}$. Do you see terms that go like $\cos^2(\omega t)$ and $\sin(\omega t)\cos(\omega t)$? Now, take a time average (over a long time window or simply over a period $T = 2\pi/\omega$) to get the time averaged energy loss (due to heat generation), i.e., $\langle \mathbf{J} \cdot \mathbf{E} \rangle$. Which part, σ_1 or σ_2, is responsible for energy loss? This is an important piece of physics.

(f) Discuss the the relative importance of σ_1 and σ_2 as frequency increases. In particular, at low frequencies, σ_1 dominates and hence energy loss is important (this is high school physics – a resistor is heated up when there is a current through it). As frequency increases, the imaginary part grows and energy loss drops! For $\omega\tau \gg 1$, show that the response is lossless! It means that a conductor (metal), while highly absorptive (energy loss) near static frequency and highly reflective (metals look shiny – see part (h)) at about 10^{14} Hz or $\hbar\omega \sim 2 - 3$ eV (optical frequencies), it becomes lossless, i.e., **transparent** at high frequencies, e.g., $\hbar\omega \sim 7 - 8$ eV. It is REAL STUFF! Many metals are transparent at high frequencies! How high should this frequency be? Check that in your answer at high frequencies, the parameter τ disappears and you have a combination ne^2/m. Now inserting a factor of ϵ_0 (the free space permittivity) and form $ne^2/m\epsilon_0 \equiv \omega_p^2$, check that it is of units of frequency squared. The frequency ω_p is called the **bulk plasma frequency**. Using n for your favorite metal (e.g. gold (or potassium) in Problem 4.1), estimate ω_p. The above discussion says that for $\omega > \omega_p$, the metal becomes transparent! **(See SQ13 for sodium.)**

(g) However, when looking at optical properties (in solid state physics, "optical" covers a wider range of frequencies than the visible range), people like to talk about **dielectric constant** or **relative permittivity**. But so far, we "think" in terms of a conductor. The above analysis shows that there is an imaginary part σ_2 that works like a dielectric, i.e., non-dissipative or no energy loss, and thus using a dielectric constant to describe a metal is not entirely unreasonable.

Let's start with a description using $\sigma(\omega)$. From the Maxwell equation:

$$\nabla \times \mathbf{H} = \mathbf{J}_{free} + \epsilon_0 \frac{\partial \mathbf{E}}{\partial t}, \tag{5}$$

using $\mathbf{J} = \sigma\mathbf{E}$ and assumes a harmonic time $e^{-i\omega t}$, show that the above equation becomes

$$\nabla \times \mathbf{H} = \sigma\mathbf{E} - i\omega\epsilon_0\mathbf{E}. \tag{6}$$

So far so good – up to here we used σ (conductivity) only. Next, we take the point of view that everything can be described instead in terms of a dielectric constant. We introduce a **complex dielectric constant** $\tilde{\epsilon}$ by imposing that the right hand side of the above equation is:

$$\nabla \times \mathbf{H} = -i\omega\tilde{\epsilon}\mathbf{E}. \tag{7}$$

Obtain an equation for $\tilde{\epsilon}/\epsilon_0$, this is the complex relative permittivity (also called dielectric constant). Technically, we impose the picture that all the currents are regarded as "displacement current".

Now, substituting $\sigma(\omega)$ for σ into your equation and using the definition of ω_p, show that

$$\epsilon_{metal}(\omega) \equiv \frac{\tilde{\epsilon}}{\epsilon_0} = 1 - \frac{\omega_p^2}{\omega(\omega + i/\tau)}. \tag{8}$$

This is the famous **Drude formula for the dielectric constant of a metal**.

(h) Write down explicitly the real $\epsilon_1(\omega)$ and imaginary parts $\epsilon_2(\omega)$ of $\epsilon_{metal}(\omega)$. Sketch them as a function of ω from $\omega \ll \omega_p$ to $\omega > \omega_p$. [Note: For many metals, $\omega_p\tau \sim 100$ or so.] You may want to plot it as $\epsilon_{metal}/\epsilon_0$ against ω/ω_p.

In general, one can define a complex refractive index as $\tilde{n} = \sqrt{\tilde{\epsilon}/\epsilon_0}$. For simplicity, let's say we can ignore $1/\tau$ in the denominator (it is called "assuming the metal to be lossless"). We then have

$$\epsilon_{metal}(\omega) = 1 - \frac{\omega_p^2}{\omega^2}. \tag{9}$$

Recall that the reflectivity R at normal incidence (see Griffith's textbook) is given by

$$R = \left|\frac{\tilde{n} - 1}{\tilde{n} + 1}\right|^2, \tag{10}$$

where $\tilde{n} = \sqrt{\epsilon_{metal}}$ is now a complex refractive index. What is R for $\omega < \omega_p$? Explain why we can use copper as a mirror. Sketch $R(\omega)$ as a function of ω (or ω/ω_p). **(See SQ13.)**

(i) (Optional: No bonus point) Some scientists prefer to work with the refractive index than the dielectric constant. Given that the dielectric constant is $\epsilon = \epsilon_1 + i\epsilon_2$, find the real and imaginary parts n_1 and n_2 of the complex refractive index $n = n_1 + in_2$.

Remarks: What we did here is part of the bigger problem of *Optical Properties of Solids*. For those interested in this subject, I would recommend the following two textbooks:
Mark Fox, *Optical Properties of Solids* (Oxford University Press 2001, 2009)
Frederick Wooten, *Optical Properties of Solids* (Academic Press 1972)
The relevant chapter (Ch.9) in Griffiths' *Introduction to Electrodynamics* provides the necessary background (see Lorentz oscillator model of dielectric constant).

4.3 **(Empty lattice approximation – Warming up)** The nearly free electron model is a way to get at the electronic band structure (see Chapter X). Conceptually, the method involves two steps. We start with the FREE ELECTRON energy dispersion relation $\epsilon^0(k)$. Note that at the free electron level, we do NOT have the idea of an atomic periodicity in mind. In Step 1, we **imagine** that **a periodic potential of infinitesimal strength** is turned on. After imposing the atomic periodicity, then ideas such as direct lattice, reciprocal lattice, 1st Brillouin zone (BZ), etc. all enter. However, due to the tiny tiny strength of the potential, the free electron energies are NOT modified, only that we can **FOLD** the free electron energy dispersion relation **into the 1st BZ**. This is the **empty lattice approximation**. Thus, the idea is that in Step 1, only the periodicity (not the strength of the potential) is considered. In Step 2, the effects of the strength of the potential is considered and band gaps may be formed. Here, we will practice Step 1.

The easiest problem is to consider a 1D system of period a (i.e. lattice constant a).

(a) In a clean (and to the right scale) diagram, draw the FREE electron energy dispersion relation (you may do this using a graphic software if you want/can). Next, consider the effect of imposing an infinitesimally weak periodic potential of period a. In another clean diagram, fold the free electron band into the 1st BZ – Show at least 4 bands (i.e., for each value of k in the 1st BZ, there should be at least 4 energies). What you get is the empty lattice approximation in a 1D system.

(b) Making use of periodicity, we can restrict k to within the 1st BZ. Take $k = 0$ (zone center), write down the energies (4 of them as shown in your figure) of the 4 states in terms of k and a reciprocal lattice vector G. Note that $\mathbf{G} = n\frac{2\pi}{a}\hat{x}$ in a 1D system, where n is an integer, i.e., $n = 0, \pm 1, \pm 2, \cdots$.

(c) Similar to (b), take $k = \frac{\pi}{2a}$. Write down the energies of the 4 states in terms of k and a reciprocal lattice vector G.

(d) Now take a value of $k \in$ 1st BZ (a value that you like). See if there is a general pattern that the energies higher than the lowest energy for a value of k can be expressed in terms of k and some G?

(e) What is the maximum energy of the lowest band? What is the minimum energy of the second lowest band? Then, list the minimum/maximum energy of each of the 4 bands shown in your figure.

Remark: (See SQ 16) So it is easy to follow the empty lattice approximation in 1D. In higher dimensional systems, the empty lattice approximation is more complicated due to the shape of the 1st BZ in higher dimensions and the possibility of having many more degeneracies (crossing of folded bands within the 1st BZ) in the 1st BZ. If you find it necessary to go through a 2D exercise, try to repeat the problem for a 2D square lattice.

4.4 **Nearly free electron model in a 1D system** – *You should make a serious attempt on this problem, as it illustrates all the basic ideas in band theory – including the nearly free electron model, semiconductor, band gaps, and effective mass.* This is a continuation of Problem 4.3 in which you did the empty lattice approximation in 1D. There are not too many band structure problems that can be done by hand. This is one that has become a standard problem in many textbooks. [Read Chapter XII class notes as self-learning, before we discuss them in class.]

Review the nearly free electron model – the key point is that the gaps are controlled by the Fourier coefficients $V(\mathbf{G})$ of the periodic potential.

Here is a one-dimensional (1D) example. Consider a 1D periodic potential. The period is a. Mathematically, the potential $V(x)$ is given by

$$V(x) = \begin{cases} \frac{1}{2}m\omega^2[b^2 - (x-na)^2], & na - b \le x \le na + b \\ 0, & (n-1)a + b \le x \le na - b \end{cases}$$

where $a = 4b$, ω is a constant.

(a) Sketch $V(x)$.

(b) Find the average of $V(x)$. How is it related to the Fourier coefficient of $V(x)$, i.e., which Fourier component corresponds to the spatial average of $V(x)$?

(c) The reciprocal lattice vectors are given by $G_n = n2\pi/a$, where $n = 0,\pm1,\pm2,\ldots$. (Why is it?) Now, evaluate the Fourier coefficient $V(G_n)$. [Hint: This involves doing an integral (in Fourier transform), which can be reduced to an integral over one unit cell. The integral can be done analytically.]

(d) Hence, give the band gap between the lowest and second bands; and the band gap between the second and the third bands.

(e) Sketch the band structure, including the lowest three energy bands.

(f) After we put the electrons into the bands, if there are only full and empty bands then the solid is a non-conductor (insulator or semiconductor); and if there is (are) partially filled band (bands), then the solid is a conductor. Given that there are 4 electrons in a unit cell, would you expect the solid to be a conductor or a non-conductor?

(g) According to part (f), which band will be the valence band and which band will be the conduction band? **The following may be slightly harder – but we have covered all the techniques in class.** We discussed the opening of the gap. Now focusing on the opening of a gap between the valence band and conduction band, derive the energy dispersion relations $E_c(k)$ for the conductor band and $E_v(k)$ for the valence band, for k in the **vicinity of the gap**. (That is to say, we want to know how the conduction band curves upwards and how the valence band curves downwards for k very close to the gap. A 2×2 matrix formalism will be useful.)

(h) While we started with the bare electron mass m in our calculation (when we do the band folding or see the Schrödinger equation), here we get a curvature different from free electron bands for the conduction and valence bands near the gap. More, we have $E(k) \sim k^2$, i.e., **parabolic** (do you see that in your results in part (g)?). Hence, electrons near the bottom of conduction band and top of valence band are **free-electron-like** but carry an effective mass m^* (Chapter XII of class notes will give a formal definition). Basically, parabolic bands can be modeled by $\hbar^2k^2/(2m^*)$. Derive analytic expressions for m^* for electrons near the bottom of conduction band and top of valence band.

(i) Hence, using the band structure to derive expressions for the velocity of electrons in the conduction and valence bands for k close to the band gap. What are the velocities at the top of valence band and bottom of conduction band? [See Chapter XII class notes.]

(j) **Don't need to do anything here! Just go through what you have done in all the parts and consolidate what you learn in this problem.**

(k) [Optional: A remark is that (for those who like to do computational problems) using the analytical form of $V(G_n)$ in part (c), one can set up the matrix problem using the Central Equation (in plane wave expansion) to any size (try it if you really have the heart to learn band theory in solid state physics), i.e., taking $n = 0$, ±1, ±2, etc. (say to ±5). Then you get a 11×11 matrix if you truncate the $\infty \times \infty$ matrix to this size. Diagonalizing the matrix will give you 11 bands for each k value in the Brillouin zone. I thought it would be quite interesting to go through the exercise.]

MID-TERM EXAMINATION
Date: 21 March 2013 (Thursday)
Time: 14:30 – 16:15 (our regular class time)
Venue: LSB C2 (our regular classroom)
Coverage: *From Chapter I to end of Chapter IX, and slightly into Chapter X (Empty Lattice Approximation) of class notes, including materials covered in Lectures, Class Notes, Problem Sets, and Sample Questions.*

Important: For every PHYS4450 Problem Set, you must attach a SIGNED copy of the academic honesty declaration form given below. It is a university policy. Homework without a signed declaration form will NOT be graded and thus will carry zero mark.

I declare that the assignment here submitted is original except for source material explicitly acknowledged, and that the same or related material has not been previously submitted for another course. I also acknowledge that I am aware of University policy and regulations on honesty in academic work, and of the disciplinary guidelines and procedures applicable to breaches of such policy and regulations, as contained in the website http//www.cuhk.edu.hk/policy/academichonesty.

Signature	**Date**
Name	**Student ID**
Course code	**Course title**