PHYS*4150: Review problems

Problem 1: Drude

a) A collision process with a relaxation τ is assumed in Drude's model for electrical conductivity in metals. Under the influence of an external electrical field, will this collision process enhance or hinder the electronic current?

b) If we want to propagate a high frequency AC signal $E(r,t) = Re(E(r,\omega)e^{-i\omega t})$ in a metal, what is the frequency condition one needs to satisfy?

c) The figure below shows a Hall effect measurement on Aluminum metal. R_H is the Hall coefficient and n is the free electron density based on a nominal chemical valence of Aluminum ($3e^-$/primitive cell). What does the result at high **H** field suggest for the conduction charge density n_0 (in unit of e^-/primitive cell)?

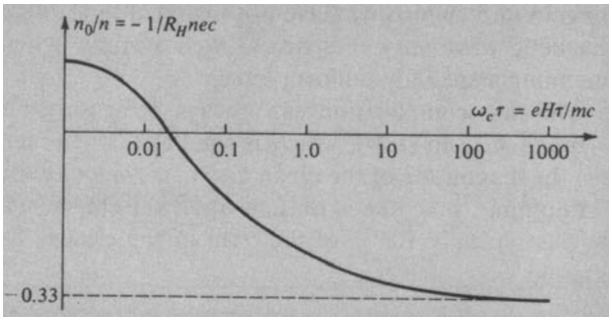


Figure 1: Hall effect in Aluminum metal.

Problem 2: Sommerfeld

a) For electronic constant volume specific heat, classically we have from the equal energy partition theorem $c_V = \frac{3}{2}nk_B$, where n and k_B are electron number density and Boltzmann's constant, respectively. Sommerfeld's free electron gas theory on the other hand predicts $c_V = \frac{\pi^2}{2}\frac{k_BT}{\varepsilon_F}nk_B$, where T and ε_F are the temperature and system Fermi energy, respectively.

i) For metals at room temperature, what is the order of magnitude for the factor $\frac{k_BT}{\varepsilon_F}$?

ii) Briefly explain the reason for the difference between the classical result and that from the Sommerfeld theory.

iii) At roughly what temperature are the values from the quantum mechanical result and the classical result close to each other?

b) Given that ε_F ranges roughly between 1.5 eV to 15 eV, estimate the corresponding range of Fermi velocity for free electron gas.

c) A rectangular piece of metal crystal has the following real space dimensions: length $L1$, width $L2$ and thickness $L3$. Suppose there are N conduction electrons in this metal, calculate the Fermi energy of the conduction electrons under the free electron gas approximation.

d) Figure 2 shows for a free electron gas the density of states per unit volume, $g(\varepsilon)$, as a function of electron energy ε. Try to answer the following from a conceptual level, without detailed calculations.

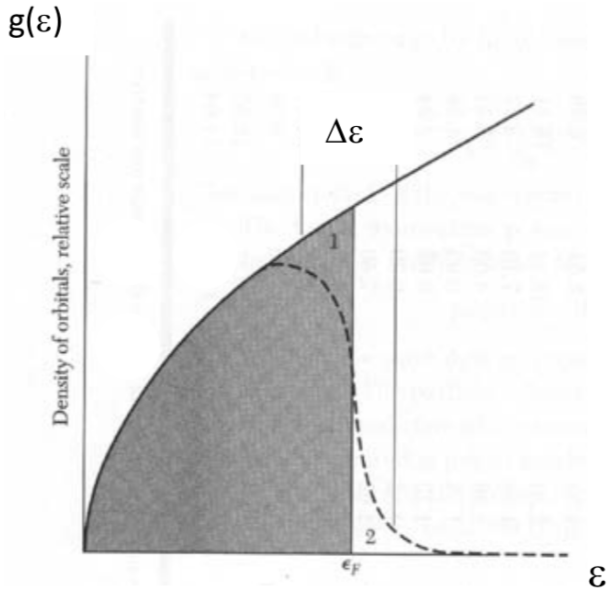


Figure 2: Free electron model density of states.

i) For $\varepsilon \sim \varepsilon_F$, indicate which curve segment (dashed or solid) corresponds to the shape of $g(\varepsilon)$ at i) $T = 0$ K and ii) $T > 0$ K, respectively.

ii) At a temperature T close to room temperature, there is a range of electron energy where the density of states deviates from that at $T = 0$ K, what is approximately this energy range $\Delta\varepsilon$?

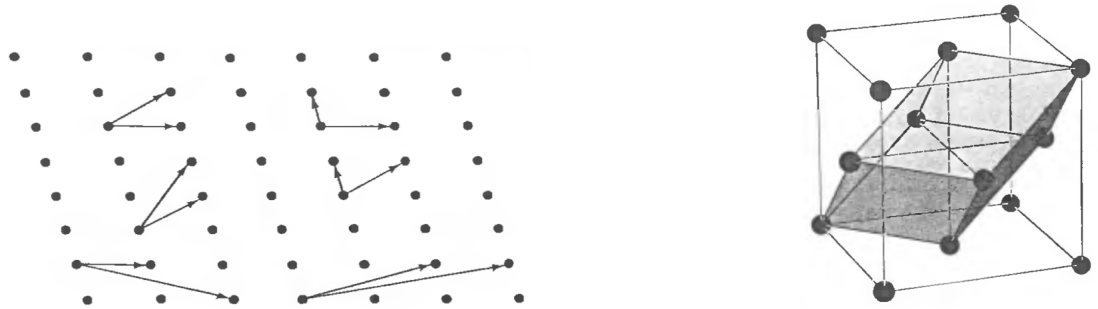
iii) Suppose the density of states per unit volume near the Fermi energy is known to be $g(\varepsilon_F)$, what is approximately the number of electrons that is in the energy range $\Delta\varepsilon$?

iv) At a temperature T close to room temperature, for the electrons in the energy range $\Delta\varepsilon$, what is approximately the thermal energy of each of them?

v) Extend the results from the above discussions and qualitatively show that at a temperature T close to room temperature the electronic specific heat c_V is linearly proportional to the temperature T in the free electron model.

Problem 3: Crystal lattice

a) Figure 3a below shows several choices of pairs of primitive vectors for a 2D Bravais lattice. Add one more pair which would be different from the ones already shown.



(a) Lattice vectors in 2D. (b) FCC unit cell.

Figure 3

b) Figure 3b shows a FCC lattice with lattice constant a, and also shown is a choice of its primitive cell (shaded volume). Make an argument to show that the shaded volume is $\frac{1}{4}a^3$.

c) For the 2D pattern shown in Fig. 4, construct a Bravais lattice to represent the repetitive pattern. How many light/dark lizards are in the primitive unit cell? What are the basis point vectors of each lizard in the unit cell (in units relative to the primitive lattice vectors)?

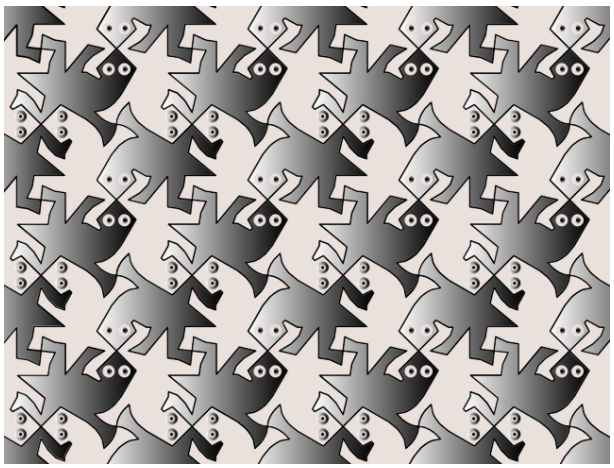


Figure 4: Lizard lattice in 2D.

d) For a two-dimensional simple rectangular lattice, what would be the shape of its Wigner-Seitz cell? How many Bravais lattice points are in the Wigner-Seitz cell?

e) What is the Bravais lattice for a sodium chloride structure?

Problem 4: Reciprocal lattice

a) What is the term for the Wigner-Seitz cell in a reciprocal lattice?

b) For a simple cubic lattice with lattice constant a, determine its reciprocal space primitive cell volume in terms of a. Do the same for a BCC and FCC lattice.

c) For (111) and (220) planes of a cubic Bravais lattice, which set of planes has a shorter d-spacing (i.e. inter-plane space)? Which one has a higher number density of Bravais lattice points?

d) If a simple cubic Bravais lattice has its lattice constant increased by a factor of 3, what would be the resulted change in the 1st Brillouin zone volume?

e) Using the conventional (cubic) FCC unit cell, determine the Miller indices for the family of planes which is indexed as (001) with respect to the *primitive* lattice vectors.

Problem 5: Diffraction

a) X-rays used for medical imaging are typically having energies on the order of 100 keV. What would be the corresponding wavelength?

b) What would be the radius of the Ewald sphere for the X-rays in (a)?

c) Which formulation of X-ray diffraction by crystal lattice is more general: Bragg or Laue?

d) In general the X-ray scattering amplitude form a sample can be expressed as the following integral:

$$Amplitude = \int_{crystal} e^{i(\mathbf{k}'-\mathbf{k})\cdot\mathbf{r}}\rho(\mathbf{r})d\mathbf{r}, \tag{1}$$

where $\mathbf{k}$ and $\mathbf{k}'$ are the incoming and scattering X-ray wave vectors, respectively, and $\rho(\mathbf{r})$ is the electron density. The integral above is over the entire crystal. Write out this Amplitude in a combination of the following terms: atomic form factor, structure factor, Bravais lattice sites; indicate explicitly for each integral or sum the ranges or the meaning.

Problem 6: Bloch's theorem

a) For a Bloch wave $\psi_k(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}}u_k(\mathbf{r})$ in a weak periodic potential, as the potential gets weaker, what kind of a period function $u_k(\mathbf{r})$ would tend to become?

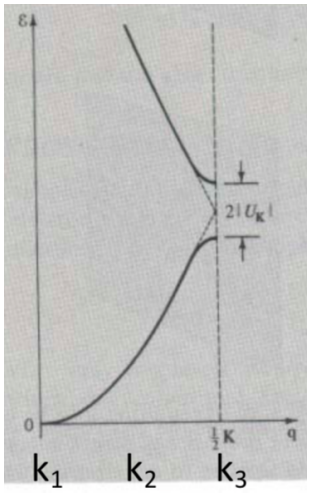
b) The reciprocal space volume for a single electron energy level $\Delta\mathbf{k}$ can be expressed as $\Delta\mathbf{k} = \frac{1}{N}\mathbf{b}_1 \cdot \mathbf{b}_2 \times \mathbf{b}_3$, where $\mathbf{b}_i$'s' are the reciprocal lattice primitive vectors. What does the quantity N represent?

c) Using Bloch theorem and noticing that $u_k(\mathbf{r}) = \sum_{\mathbf{K}} c_{\mathbf{k}-\mathbf{K}} e^{-i\mathbf{K}\cdot\mathbf{r}}$ ($\mathbf{K}$ is a reciprocal lattice vector), show that the electron energy band function is periodic in $\mathbf{K}$, i.e. $\varepsilon_{\mathbf{k}+\mathbf{K}} = \varepsilon_{\mathbf{k}}$.

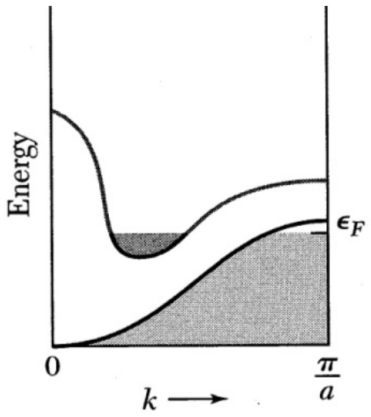
Problem 7: Electrons in a weak periodic potential

a) For a monatomic metallic crystal with N atoms (one per Bravais lattice site) in a simple square lattice (2D), if the valence is 3 for the metal, determine if the 2nd Brillouin zone is entirely within the Fermi circle.

b) In the 1D electron energy band diagram shown in Figure below, for the first band indicate which k value would correspond a higher average electron velocity, $k_1 = 0$, $k_2 = 0.25K$ or $k_3 = 0.5K$? Why? (K is the primitive reciprocal lattice vector.)



(a) 1D nearly free electron energy bands.



(b) Unknown material band structure.

Figure 5: Nearly-free electron model.

c) What is the mathematical definition of the quantity U_k in Fig. 5a? For a 1D periodic potential $V(x) = -\sin\frac{2\pi}{a}x$, what is the corresponding $U_{\frac{2\pi}{a}}$?

d) Identify the type of material for which the band structure is shown in Fig. 5b. Explain.

Problem 8: Dynamic lattice

a) In the harmonic lattice approximation, what physical significance do the terms $\varphi^0(n', n)$ have?

b) Write the Hamiltonian in the harmonic lattice approximation for a 1D monatomic lattice assuming 1st, 2nd, and 3rd nearest-neighbour interactions. Use different parameters for each interaction type.

c) Using the *dynamical matrix*, determine the dispersion relations for a 1D monatomic lattice with alternating force constants (see example on page 433 in A&M). Plot the results.

d) Compare typical energies and effective momenta of phonons and photons. For photons consider optical (i.e. visible light) frequencies; for phonons consider frequencies in the 10 THz region. Make reasonable assumptions where required.

e) What is a fundamental difference in the filling of electron energy levels vs. phonon energy levels?