Due Date: 31 March
Reading Assignment: Sapoval and Hermann, 2.2-2.4, Chapter 4

Problems:

1. This a famous problem that shows how far the free electron model can be pushed to describe actual solids.
   a). Write the single particle three dimensional Hamiltonian for an electron that experiences no force.

   b). Write the general form of the wavefunctions that are eigenstates of the three dimensional momentum operator.

   c). Show that the momentum eigenstates are also eigenstates of the Hamiltonian. What is the relation between the momentum and energy eigenvalues?

   d). Impose periodic boundary conditions on a cube of side $L$. Illustrate the allowed values of $k$, where $k$ is the wavevector of the eigenfunctions.

   e). Compute the number of eigenstates that have energy between $E$ and $E + dE$. Include spin degeneracy. Assume that $E$ and $E + dE$ are large enough that there is a very large number of such states.

   f). Compute $n(E)$ and $N(E)$, the density of states and the density of states per unit volume of the cube.

   h). Fill the above cube with $N$ electrons. Find the maximum energy level occupied under these conditions. This is the electrochemical potential (or Fermi Energy) at $T=0K$.

   i). Compute the total energy of the electron gas at $T=0K$.

   j). Compute the pressure exerted by the electrons, $P = -\left(\frac{\partial E}{\partial V}\right)_{T,N}$, where $E$ now is the total energy of the electron gas, $V$ its volume, $T$ the temperature and $N$ the number of particles.

   k). Compute the Bulk Modulus, defined by $B = -V\left(\frac{\partial p}{\partial V}\right)_{T,N}$, at $T=0K$.

   l). Compute a numerical value for $B$ assuming that $N/V$ is $2.65 \times 10^{22}$ cm$^{-3}$. This is the density of valence electrons in sodium, assuming each atom contributes one valence electron. Compare with the measured value of $6.81 \times 10^{10}$ dynes cm$^{-2}$.
2. Find and neatly sketch the BCC $|s>$ orbital energy bands along the directions parallel to the unit cube edge, along the unit cube diagonal, and along the unit cube face. Assume the cube side is $a$.

3. Crystal Structure

While two-dimensional crystals are easy to draw on the board and to discuss, the real world is three dimensional. However, there are still several examples of two-dimensional lattices that show up in a three-dimensional world. The most relevant example in our case is the surface of a semiconductor which we may consider a two-dimensional array of points existing in three-dimensional space.

On the test, we found the reciprocal lattice for a two-dimensional crystal. In order to facilitate calculations, I suggested you “...assume the lattice has a third primitive translation vector $c\hat{z}$ coming out of the page.” However, by letting $c$ go to infinity, we approach a true two-dimensional structure or, in practice, a crystalline surface.

a) Describe the effect of letting $c$ approach infinity on the reciprocal lattice. Give a description of the actual reciprocal lattice of a two-dimensional array of points in three-dimensional space.

b) We constructed primitive cells in real space and the first Brillouin Zones in reciprocal space and using the Wigner-Seitz construction - the volume bounded by the perpendicular bisectors to the nearest neighbors. The second Brillouin zone can be similarly defined - the volume between the perpendicular bisectors to the second nearest neighbors and the first Brillouin Zone and similarly for the third and fourth zones.

Accurately sketch the second and third Brillouin zones for the following real space lattice. Be careful to identify the second and third nearest neighbors. These zones will consist of more than one piece.

c) Assume that the free electron model applies and complete the $E$ vs. $k$ diagram for two directions along the zone edge and along the zone diagonal OUTSIDE THE FIRST BRILLOUIN ZONE, up to and including the third Brillouin zone. By using the reduced zone scheme, complete the diagram below by labeling the contributions from the first, second and third Brillouin zones:
d) Using what you deduced in part a) and b) tell me the three dimensional Fourier transform of a two dimensional array of lines?

4. Find the four dimensional free electron density of states per unit 4D volume. Assume the differential 3D volume element in 4D space is $8\pi^3 dr$.

5. An electron in a one dimensional, single atom basis material is under the influence of an electric field. How large must the electric field be in order for the electron to completely traverse the first Brillouin zone without scattering if the scattering time is about $4.14 \times 10^{-12}$ seconds. The distance between the atoms is $2.5\text{Å}$

6. Imagine an LCAO band for a simple cubic structure (with cube edge a) given by

$$E(k) = -E_0(\cos k_x a + \cos k_y a + \cos k_z a)$$

Let an electron at rest ($k=0$) feel a uniform, constant electric field, $\mathbf{E}$.

a) Find the trajectory in real space. This can be done by specifying $x(t)$, $y(t)$ and $z(t)$.

b. Sketch the trajectory in the x-y plane if $\mathbf{E} = \mathbf{E}_0 \mathbf{e}$ oriented in the [210] direction.