There are 4 problems.

Problem#1 (7 points)

(i)   Write down the energy $\varepsilon(k_x,k_y)$ of an electron moving in a 2-dimensional square lattice (lattice constant a) in terms of the intrasite (-α) and nearest neigh hopping parameters ($-\gamma$) as a function of k_x, k_y, the x and y components of the electron wave vector k.

$$\varepsilon(k_x,k_y) = -\alpha - 2\gamma\left(\cos k_x a + \cos k_y a\right)$$

(ii)   What is the effective mass of an electron with wave vector close to (π/a,0) of the 1st Brillouin zone if it is (a) moving along the x direction or (b) moving along the y direction?

$$For\ (k_x,k_y) = (\pi/a, 0);\ \varepsilon(\pi/a,0) = -\alpha$$

$$For\ (k_x,k_y)\ near\ (\pi/a,0);\ k_y\ and\ K_x = \frac{\pi}{a} - k_x\ are\ small$$

$$\varepsilon(k_x,k_x) \approx -\alpha - \gamma K_x^2 a^2 + \gamma k_y^2 a^2 = -\alpha + \frac{\hbar^2}{2m_x^*}K_x^2 + \frac{\hbar^2}{2m_y^*}k_y^2$$

$$m_x^* = -\frac{\hbar^2}{2\gamma a^2};\ Negative\ effective\ mass\ along\ x-direction$$

$$m_y^* = +\frac{\hbar^2}{2\gamma a^2};\ Positve\ effective\ mass\ along\ y-direction$$

Note (as discussed in the class)

$$For\ (k_x,k_y)\ near\ (0,0);\ k_y\ and\ k_x\ are\ small$$

$$m_x^* = m_y^* = +\frac{\hbar^2}{2\gamma a^2}$$

$$For\ (k_x,k_y)\ near\ (\pi/a,\pi/a);\ K_y = \frac{\pi}{a}k_y\ and\ K_x = \frac{\pi}{a} - k_x\ are\ small$$

$$m_x^* = m_y^* = -\frac{\hbar^2}{2\gamma a^2}$$

Problem#2 (15 points)

Consider a three dimensional crystalline lattice formed out of Cu and Zn atoms. The Cu atoms form a cubic lattice with lattice constant a. The Zn atoms are at the center of the cube.

(i)   What is the Bravais lattice and what are the primitive lattice vectors?

CUBIC

The primitive lattice vectors are: $\vec{a}_1 = a(1,0,0); \vec{a}_2 = a(0,1,0); \vec{a}_3 = a(0,0,1)$

The basis vectors are: $\vec{r}_1 = a(0,0,0); \vec{r}_2 = a\left(\frac{1}{2},\frac{1}{2},\frac{1}{2}\right)$

(ii)   What are the primitive vectors ($\vec{b}_1, \vec{b}_2, \vec{b}_3$) of the reciprocal lattice?

$$\vec{b}_1 = \frac{2\pi}{a}(1,0,0); \vec{b}_2 = \frac{2\pi}{a}(0,1,0); \vec{b}_3 = \frac{2\pi}{a}(0,0,1)$$

(iii)   What is the volume per Cu atom?

$$V_{Cu} = a^3$$

(iv)   Write down the structure factor $S_{\vec{G}}$, associated with the reciprocal lattice vector $\vec{G} = v_1\vec{b}_1 + v_2\vec{b}_2 + v_3\vec{b}_3$ in terms of the atomic form factors f_{Cu} and f_{Zn}.

$$S_{\vec{G}} = f_{Cu}e^{i\vec{G}.\vec{r}_1} + f_{Zn}e^{i\vec{G}.\vec{r}_2} = f_{Cu} + f_{Zn}e^{i\pi(v_1+v_2+v_3)}$$

(v)   If Cu and Zn atoms randomly occupy every lattice site then the form factor associated with every lattice site can be assumed to be the same (average of the two form factors). In this case which Bragg spots will vanish?

$$f_{Cu} = f_{Zn} = \bar{f}$$
$$S_{\vec{G}} = \bar{f}(1 + e^{i\pi(v_1+v_2+v_3)})$$

Bragg spots will vanish when $v_1 + v_2 + v_3 = Odd$

Problem#3 (10 points)

Consider a two-dimensional electron system where the energy of an electron is given by
$$\varepsilon_{\vec{k}} = \hbar v\,k\,,$$

v is the speed of the electrons and $\vec{k}$ is the electron wave vector. Such an approximation is good for extremely relativistic electrons.

  (i)   Calculate the density of states $D(\varepsilon)$ as a function of area A, $\hbar v$, and energy ε. Include the spin degeneracy factor. Plot $D(\varepsilon)$ as a function of ε.

$$D(\varepsilon)d\varepsilon = 2\,\frac{2\pi k dk}{\left(2\pi/L\right)^2}\,;\; \varepsilon = \varepsilon_{\vec{k}} = \hbar v k\,; d\varepsilon = \hbar v dk$$

$$D(\varepsilon) = \frac{A}{\pi}\left(\frac{1}{\hbar v}\right)^2 \varepsilon$$

The density of states varies linearly with energy.

  (ii)   Calculate the Fermi energy of this system if the electron density is $10^{12}\,cm^{-2}$. Use $v = 10^8\,cm/s$.

$$N = \int_0^{\varepsilon_F} D(\varepsilon)d\varepsilon \Rightarrow \frac{A}{\pi}\left(\frac{1}{\hbar v}\right)^2 \varepsilon_F^2/2$$

$$\varepsilon_F = \hbar v\sqrt{2\pi(N/A)} = 2.63 x 10^{-20}\,J = 0.164\,eV$$

Problem#4. (8 points)

The conduction electrons in a metal can be modeled as an ideal Fermi gas with fermion effective mass m^*.

(i)   How does the electronic heat capacity C_V vary with temperature, for $T \ll T_F$, the Fermi temperature?

$$C_{el} \sim \gamma T; \quad \gamma \sim D(\varepsilon_F) \sim \frac{N}{\varepsilon_F}$$

(ii)   If the effective mass increases by a factor of 10 (say due to the effect of strong crystalline potential), what will be the change in C_V at a fixed T?

$$\varepsilon_F \sim \frac{1}{m^*} \rightarrow \gamma \sim m^*$$

The heat capacity will increase by a factor of 10.

(iii)   Will the Pauli spin susceptibility χ_{Pauli} (at low T) associated with these electrons change? If so, by what factor and why?

Since χ_{Pauli} and γ are both proportional to the density of states at the Fermi energy $D(\varepsilon_F)$, their ratio is a universal constant, Wilson ratio. Therefore χ_{Pauli} will also increase by a factor of 10.