Q 1) Prove:

(a) than an infinite point lattice is only capable of showing 2, 3, 4, or 6-fold type rotational symmetry;

(b) the Weiss zone law, i.e. if [*uvw*] is a zone axis and (*hkl*) is a face in the zone, then $hu + kv + lw = 0$;

(c) that in the cubic system the direction [hkl] is parallel to the face-normal (hkl);

(d) that in the cubic system the angle ϕ between the face-normals ($h_1k_1l_1$) and ($h_2k_2l_2$) is given by

$$\cos\phi = \frac{(h_1h_2 + k_1k_2 + l_1l_2)}{\sqrt{[h_1^2 + k_1^2 + l_1^2}\sqrt{[h_2^2 + k_2^2 + l_2^2}}$$

(e) that, when using Miller-Bravais indices (*hkil*), $h + k + i = 0$

Ans 1)

(a) Let's consider a regular polygon with n sides. Each vertex acts like a rotation point. According to trigonometry of a regular polygon, interior angle subtended by two successive arms of a regular polygon is always $\pi - \frac{2\pi}{n}$ radians. If m faces meet at vertex, then equation that satisfies this condition is:

$$\pi - \frac{2\pi}{n} = \frac{2\pi}{m}$$

=> $\frac{1}{n} + \frac{1}{m} = \frac{1}{2}$

=> m and n can only be 3, 4 or 6. It implies that a plane can only be filled with convex or regular polygons which are either equilateral triangles, squares, or hexagons (i.e. n = 3, 4, or 6)

Note: **n cannot be 2**. It means there's no plane and polygon is actually a straight line. And a straight line cannot fill any plane. It needs to have at least 3 points to form a closed structure and fill the plane.

(b) Unit vector passing through the face plane (hkl) is nothing but

$$\hat{P} = \frac{h}{x}\hat{i} + \frac{k}{y}\hat{j} + \frac{l}{z}\hat{k}$$

and the Weiss zone axis vector for its direction [uvw] is

$$\vec{W} = ux\hat{i} + vy\hat{j} + wz\hat{k}$$

But these are actually perpendicular, and must satisfy the equation $\hat{P}\,.\vec{W} = 0$ (i.e. dot product)

i.e. $\left(\frac{h}{x}\hat{i} + \frac{k}{y}\hat{j} + \frac{l}{z}\hat{k}\right).ux\hat{i} + vy\hat{j} + wz\hat{k} = 0$

=> $hu + kv + lw = 0$

(c) In the cubic system, equation of unit vector of the plane becomes

$\hat{P} = \frac{h}{a}\hat{i} + \frac{k}{a}\hat{j} + \frac{l}{a}\hat{k}$, where a is the lattice parameter

The direction vector for (hkl) is

$\vec{D} = ha\hat{i} + ka\hat{j} + la\hat{k}$

Their cross product is $\hat{P}X\vec{D} = (\frac{h}{a}\hat{i} + \frac{k}{a}\hat{j} + \frac{l}{a}\hat{k})X(ha\hat{i} + ka\hat{j} + la\hat{k})$, which is equal to 0. It implies that they are parallel to each other.

(d) Let us consider the unit vector passing through $h_1k_1l_1$ and $h_2k_2l_2$ be $\hat{V}_1 = d_1(h_1\hat{i} + k_1\hat{j} + l_1\hat{k})/a_1$ and $\hat{V}_2 = d_2(h_2\hat{i} + k_2\hat{j} + l_2\hat{k})/a_2$ respectively, where $\mathbf{d_1}$ and $\mathbf{d_2}$ are the interplanar distances and $\mathbf{a_1}$ and $\mathbf{a_2}$ are the lattice parameters. Their cross product is $\hat{V}1.\hat{V}2 = |\hat{V}1||\hat{V}2|\cos\phi$, but their mod is equal to 1 as they are unit vectors. Hence, the equation reduces to $\hat{V}1.\hat{V}2 = \cos\phi$

Also, interplanar distance is related to lattice parameter and position vector as

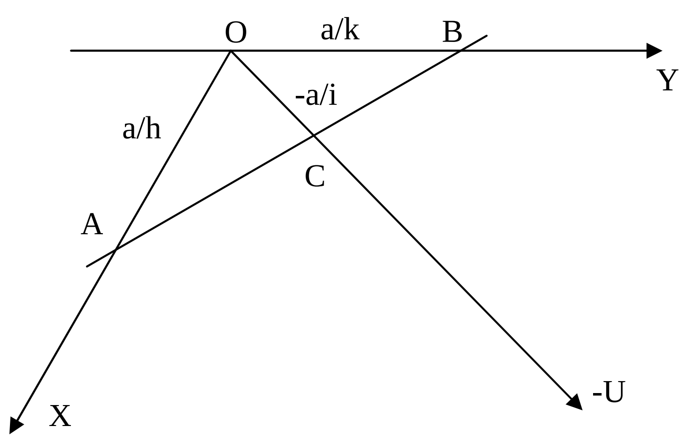
$$d = \sqrt{\frac{a^2}{h^2 + k^2 + l^2}}$$

Hence, $\cos\phi = d_1d_2(h_1h_2 + k_1k_2 + l_1l_2)/a_1a_2$

Replacing a_1 and a_2, and the equation reduces to

$$\cos\phi = \frac{(h_1h_2 + k_1k_2 + l_1l_2)}{\sqrt{h_1^2 + k_1^2 + l_1^2}\sqrt{h_2^2 + k_2^2 + l_2^2}} \text{ ….. proved}$$

(e)



In the aforedrawn figure, Area of triangle OAB is equal to sum of areas of triangles of OAC and OCB. From trigonometry we know that area of triangle is ½ ab sinC (where a and b are the lengths of the sides of triangle and C is angle subtended between those sides. Hence,

$-\frac{1}{2}\frac{a}{h}\frac{a}{i}\sin AOC - \frac{1}{2}\frac{a}{k}\frac{a}{i}\sin BOC = \frac{1}{2}\frac{a}{h}\frac{a}{k}\sin AOB$, sin AOC = sin BOC = sin AOB *

=> $\frac{-1}{hi} + \frac{-1}{ki} = \frac{1}{hk}$

=> $h + k + i = 0$ ………….. proved

* (Note = AOC = BOC = 60^o and AOB = 120^o, also sin 120^o = sin 60^o)

Q 2) Derive an expression for the Fermi energy of a free electron metal at zero temperature. Using the data given, and any other constants, evaluate the Fermi energy of the alkali metals.

	Li	Na	K	Rb	Cs
Density, gcm^{-3}	0.534	0.971	0.86	1.53	1.87
Atomic weight	6.939	22.99	39.102	85.47	132.905

How would you measure the Fermi energy experimentally for these metals?

Ans 2) Fermi energy is defined as the highest energy occupied by an electron at absolute zero.

According to Fermi-Dirac statistics, the probability that a particle (fermion) will have energy (E) is given by

$f(E) = \frac{1}{e^{(E-E_F)/K_\beta T} + 1}$, and at absolute zero its value is 1 -- (1)

Suppose the volume (V) contains N_e electrons. Then,

$N_e = \int_0^\infty g(E) f(E) dE$, but $f(E)$=1 from equation 1. The equation reduces to:

$N_e = \int_0^\infty g(E) dE$, but $g(E) = \frac{Vm}{\pi^2 \hbar^3}\sqrt{2mE}$

$$\Rightarrow N_e = \int_0^\infty \frac{Vm}{\pi^2 \hbar^3}\sqrt{2mE}\, dE$$

$$\Rightarrow N_e = \frac{V\sqrt{2m^3}}{\pi^2 \hbar^3}\int_0^{E_F}\sqrt{E}\, dE$$

$$\Rightarrow N_e = \frac{V\sqrt{2m^3}}{\pi^2 \hbar^3}\frac{2}{3}E_F^{3/2}$$

$$\Rightarrow E_F = \frac{\hbar^2}{2m}\left(\frac{3\pi^2 N_e}{V}\right)^{2/3}$$

Q 3) Derive an expression for the ratio κ/σ of the thermal and electrical conductivities of a free-electron metal. Calculate the value of the Lorentz number

$$L = \frac{\kappa}{\sigma T}$$

Where T is the absolute temperature. Explain the discrepancy between the calculated value and the following measured values of L for sodium at low temperatures.

T, ^oK	10	20	30	60
L, W ohm deg^{-2}	1.37×10^{-8}	0.7×10^{-8}	1.0×10^{-8}	1.2×10^{-8}

Ans 3)

Thermal conductivity (κ) = $\frac{1}{3m}\pi^2 n k_\beta^2\, T\tau$

Electrical conductivity (σ) = $\frac{ne^2\tau}{m}$

Using these two equations we can derive an expression for the ratio κ/σ, which is

$$\Rightarrow \frac{\kappa}{\sigma} = \frac{\pi^2\kappa_\beta^2}{3e^2}T \quad \text{--- (1)}$$

$\frac{\kappa}{\sigma} = \frac{\pi^2}{3}\left(\frac{k_\beta}{e}\right)^2 T$, it implies that $\frac{\kappa}{\sigma} \propto T$

or $\frac{\kappa}{\sigma} = LT$, where $L = \frac{\pi^2}{3}\left(\frac{k_\beta}{e}\right)^2$, which is called as Lorentz number. Its value can be easily calculated by substitution the values of k_β and e. (k_β is 1.3807×10^{-23} and e is 1.6×10^{-19})

$$L = \frac{\pi^2}{3}\left(\frac{k_\beta}{e}\right)^2 \Rightarrow L = \frac{\pi^2}{3}\left(\frac{1.3807x10^{-23}}{1.6x10^{-19}}\right)^2$$

$\Rightarrow L = 2.45x10^{-8}$ W-ohm/K^2

Lorentz number equation is $L = \frac{\pi^2}{3}\left(\frac{k_\beta}{e}\right)^2$, which doesn't depend on Temperature

i.e. Lorentz number is temperature-independent and its value depends on the values of Boltzmann constant and electronic charge. But in reality Lorentz number depends on the relaxation processes for electrical and thermal conductivity being the same, which is not true for all the temperatures, and because of various assumptions taken (according to Drude's theory), there is a discrepancy between the calculated values and the measured values.

Q 4) Assuming that silver is a monovalent metal with a spherical Fermi surface, calculate the following quantities:
(i) Fermi energy and Fermi temperature
(ii) Radius of the Fermi surface
(iii) Fermi velocity
(iv) Cross-sectional area of the Fermi surface
(v) Cyclotron frequency in a field of 5000 oersted
(vi) Mean free path of electrons at room temperature and near absolute zero
(vii) Orbital radius in a field of 5000 oersted
(viii) Length of the side of the cubic unit cell
(ix) Lengths of the first two sets of reciprocal lattice vectors in k-space
(x) Volume of the Brillouin zone

Density of silver = 10.5 g cm^{-3}
Atomic weight = 107.87 g
Resistivity = 1.61 x 10^{-6} ohm cm at 295°K and 0.0038 x 10^{-6} ohm cm at 20°K

Ans 4) For silver $\frac{r_s}{a_0}$ = 3.02 (referred page 36, Ashcroft/Mermin)

(i) Fermi energy $\varepsilon_F = \frac{50.1eV}{(r_s/a_0)^2}$ and Fermi temperature $T_F = \frac{58.2}{(r_s/a_0)^2} x10^4 K$

=> Fermi energy ε_F is 5.493 eV and Fermi temperature T_F is 6.381 x 10^4 K

(ii) Radius of the Fermi sphere $\kappa_F = \frac{3.63}{r_s/a_0}$ Å^{-1}

=> Radius of the Fermi sphere κ_F is 1.201 Å^{-1}

(iii) Fermi velocity $v_F = \frac{4.20}{(r_s/a_0)} x10^8 cm/\sec$

=> Fermi velocity v_F is 1.39 x 10^8 cm/sec

(iv) Cross-sectional area of the Fermi surface $A = 4\pi\kappa_F^2$ Å^{-2}

=> Cross-sectional area of the Fermi surface A is 18.125 Å^{-2}

(v) Cyclotron frequency in a field of 5000 oersted

=> ν_c = 2.8H x 10^6 Hz = 14 x 10^9 Hz or 14 TeraHz

(vi) Mean free path of electrons at room temperature and near absolute temperature

=> Mean free path is $l = 92\,\mathring{A}\,X\left[(r_s/a_0)^2/\rho_\mu\right]$
=> l_{RT} = 521.17 Å and l_{NAZ} = 22.08 μ
(RT is Room temperature and NAZ is Near Absolute Zero)

(vii) Orbital radius in a field of 5000 oersted

$\omega_c = eH/mc$, and $v = r\omega_c$

=> ω_c = 2.9 x 10^6 s^{-1} and r = 103.44 m

(viii) Length of the side of the cubic cell

Given the density of Silver (10.5 gcm^{-3}) and Atomic weight (107.87 amu)

Atomic weight = 107.87 x 1.66 x 10^{-24} g = 1.79 x 10^{-22} g

Density of silver = 10.5 = mass of one atom/volume of one atom = 1.79 x $10^{-22}/(4\pi r^3/3)$

=> r^3 = 4 x 10^{-24}, and r = 1.588 Å

As Silver is a monovalent element, lattice parameter is $2\sqrt{2}$ times of radius

=> lattice parameter (a) = 4.46 Å

(ix) Lengths of the first two sets of reciprocal lattice vectors in k-space

It's nothing but $2\pi/a$

=> lengths = 1.409 $Å^{-1}$ each

(x) Volume of the Brillouin zone

Volume of Brillouin zone is nothing but the volume of reciprocal lattice in k-space

i.e. $V_B = (2\pi)^3/V$, where V is the volume of the unit cell i.e. a^3

=> $V_B = 8\pi^3/V$, and V is 88.72 $Å^{-3}$

=> V_B = 2.796 $Å^3$

Q 5) Show that the mean energy per particle at 0^oK for electrons obeying Fermi-Dirac statistics is

$$\frac{3}{5}E_F(0),$$

Where $E_F(0)$ is the Fermi energy at T = 0. Assuming the value of this quantity at a finite temperature is

$$\frac{3}{5}E_F(0)\left[1+\frac{5\pi^2}{12}\left(\frac{kT}{E_F(0)}\right)^2\right]$$

Find the value of the ratio $(C_v)_{FD}/(C_v)_{Cl}$ for an electron gas with Fermi energy 7 eV, where $(C_v)_{FD}$ is the specific heat of a gas of particles obeying Fermi-Dirac statistics and $(C_v)_{Cl}$ is the specific heat of a gas obeying classical statistics.

Ans 5)

Total energy of electrons at 0^oK can be expressed as:

$E_{total} = \int Eg(E)dE$ … equation (1)

We know that $g(E) = \frac{Vm}{\pi^2\hbar^3}\sqrt{2mE}$

Thus equation (1) reduces to

$$E_{total} = \int E\frac{Vm}{\pi^2\hbar^3}\sqrt{2mE}dE$$

$$E_{total} = \frac{\sqrt{2m^3}V}{\pi^2\hbar^3}\int_0^{E_F} E\sqrt{E}dE$$

$$E_{total} = \frac{\sqrt{2m^3}V}{\pi^2\hbar^3}\int_0^{E_F} E\sqrt{E}dE$$

$$E_{total} = \frac{\sqrt{2m^3}V}{\pi^2\hbar^3}\frac{2}{5}E_F^{5/2} \text{ ----- (equation 2)}$$

But we know that at absolute zero Fermi energy expression is:

$$E_F = \frac{\hbar^2}{2m}\left(\frac{3\pi^2N_e}{V}\right)^{2/3} \text{ (proved earlier, refer solution to problem number 2)}$$

$$E_F^{3/2} = \frac{\hbar^3}{(2m)^{3/2}}\left(\frac{3\pi^2N_e}{V}\right) \text{ ---- equation (3)}$$

Equation 2 can re-written as

$$E_{total} = \frac{m^3V}{\pi^2\hbar^3}\frac{2^{3/2}}{5}E_F^{3/2}E_F$$

$$E_{total} = \frac{m^3V}{\pi^2\hbar^3}\frac{2^{3/2}}{5}\frac{\hbar^3}{(2m)^{3/2}}\left(\frac{3\pi^2N_e}{V}\right)E_F$$