Physics 601

HW 3 - Solutions

1. Chemical Potential of 2D Electrons.

$$N = \int_0^\infty \frac{d\varepsilon \quad g(\varepsilon)}{e^{(\varepsilon-\mu)/K_B T} + 1}$$

$$g(\varepsilon) = 2 \frac{dN}{d\varepsilon} = 2 \frac{dN}{dk} \frac{dk}{dE}$$

2d $$N(k) = \frac{\pi k^2}{\left(\frac{2\pi}{L}\right)^2} = \frac{A\pi k^2}{4\pi^2} = \frac{A k^2}{4\pi}$$

$$\frac{dN}{dk} = \frac{Ak}{2\pi}$$

$$E = \frac{\hbar^2 k^2}{2m} \Rightarrow \frac{dE}{dk} = \frac{\hbar^2 k}{m}$$

$$g(\varepsilon) = \cancel{2} \frac{A\cancel{k}}{\cancel{2}\pi} \frac{m}{\hbar^2 \cancel{k}} = \frac{Am}{\pi\hbar^2}.$$

Then in two dimensions we have

$$n = \frac{m}{\pi\hbar^2}\int_0^\infty \frac{d\varepsilon}{e^{\beta(\varepsilon-\mu)}+1} = \frac{m}{\pi\hbar^2}\left(-\frac{1}{\beta}\right)\int_0^\infty \frac{e^{-\beta(\varepsilon-\mu)}(-\beta)\,d\varepsilon}{1+e^{-\beta(\varepsilon-\mu)}}$$

$$\Downarrow$$

$\beta \equiv \frac{1}{k_B T}$

$$n = -\frac{m}{\pi\hbar^2\beta}\left\{\ln\left(1+e^{-\beta(\varepsilon-\mu)}\right\}\right]_0^\infty$$

$$n = -\frac{m}{\pi\hbar^2\beta}\left\{0-\ln\left(1+e^{\beta\mu}\right)\right\}$$

$$\frac{\pi\hbar^2\beta n}{m} = \ln\left\{1+e^{\beta\mu}\right\} \Rightarrow \beta\mu = \ln\left\{e^{\frac{\pi\hbar^2\beta n}{m}}-1\right\}.$$

$$T \ll \mu \Rightarrow e^{\frac{\pi\hbar^2\beta n}{m}} \gg 1$$

(T low)

$$\Downarrow$$

$$\frac{\mu}{\cancel{kT}} \Rightarrow \frac{\pi\hbar n}{m\cancel{kT}} \Rightarrow \boxed{\mu = \frac{n\hbar\pi}{m}}$$

Independent of T

$T \ll \mu$ (T low).

2. Madelung's Rule

a) Atomic filling configuration for W $(Z = 74)$ - Tungsten

$\# e's = 2(2l+1)$.

n	s	p	d	f	g	
1	2					2
2	2	6				4
3	2	6	10			12
4	2	6	10	14		20.
5	2	6	10	14	16	38.
6	2					56
			take $4e^-$s			70

$\tilde{n} \equiv n + l$

$$[W] = \underbrace{1s^2}_{1}\ \underbrace{2s^2}_{2}\ \underbrace{2p^6\ 3s^2}_{3}\ \underbrace{3p^6\ 4s^2}_{4}\ \underbrace{3d^{10}\ 4p^6\ 5s^2}_{5}$$

$\tilde{n}$

$$\underbrace{4d^{10}\ 5p^6\ 6s^2}_{6}\ 4f^{14}\ 5d^4$$

h) Element 118 is a noble gas → what is the atomic # of the next one.

n	s	p	d	f	g	
4	2	6	10	14 ←	70	
5	2	6	10	14	18	
6	2	6 118	10	14	18	22
7	2	6	10	14	18	
8	2	6				

88
118

Element 118 full up to $7p^6$

Next noble gas full up to $8p^6$

We must do the addition

$118 + 2 + 18 + 14 + 10 + 6 = 118 + 50 = 168$

$\boxed{\text{Next noble gas } Z = 168}$

3. Chemical Bonding

(a) Five different types of bonding and atoms where expected to occur.

(i) Ionic

Electron transfer from one atom to another ⇒ ions have electrostatic interaction

Occurs between elements w/ different electronegativities (.eg I–$\underline{\text{VII}}$ compounds like NaCl)

(ii) Covalent

Sharing of electron by the two atoms in the bond

Occurs between elements of very similar electronegativities or in solids of one element
(two examples : diamond (C) or GaAs – $\underline{\text{III}}$ – $\underline{\text{V}}$ compound)

(iii) Metallic

Delocalization of valence electrons throughout solid

L and middle of periodic table.

(iv) Van der Waals.

Dipolar interaction w/ no electron transfer.

Noble gas solids, Solids composed of nonpolar molecules.

(v) H bond

H is bound to one atom but attracted to another – quite weak but long-ranged.

Very important in biological molecules.
(also in ice and more generally in different phases of H_2O).

(b) Van der Waals forces.

The van der Waals force between two atoms (or molecules) results from the interaction of their dipole moments, either permanent or fluctuating. If one atom has a dipole moment $\vec{p}_1$ in the $\hat{z}$ direction, a second one will sense an electric field

$$\vec{E} = -\frac{p_1}{4\pi\varepsilon_0 r^3}\hat{z}$$

and will then develop a dipole moment $\vec{p}_2 = \chi\vec{E}$. The potential energy of these two dipoles is then

$$U \propto -\frac{|p_1||p_2|}{r^3} \propto -\frac{p_1^2 \chi E}{r^3} \propto -\frac{p_1^2\chi}{r^6}$$

Therefore $\boxed{F = -\frac{dU}{dr} \propto \frac{1}{r^7}}$ and is <u>attractive</u>.

4. a) $T=0$ Average $KE/e = \frac{3}{5} E_F$

$$= \frac{\frac{3}{5}\frac{\hbar^2}{2m}(3\pi^2 n)}{\frac{me^4}{2\hbar^2}} \qquad 1\ Ry$$

$$= \frac{3}{5}\frac{\hbar^4}{m^2e^4}(3\pi^2 n)^{2/3}$$

$$= \frac{3}{5} a_H^2 \left(\frac{3\pi^2 \cdot 3}{4\pi r_0^3}\right)^{2/3} \qquad a_H = \frac{\hbar^2}{me^2}$$

$$= \left(\frac{3}{5}\right)\left(\frac{9\pi}{4}\right)^{2/3}\frac{1}{r_s^2} \qquad \frac{4\pi r_0^3}{3} = \frac{1}{n}$$

$$\langle KE\rangle/e = \frac{2.21}{r_s^2} \qquad r_s = \frac{r_0}{a_H}$$

b) Coulomb energy

$$U_c^{in} = e \int_0^{r_0} \frac{\rho}{r} \, 4\pi r^2 \, dr = -\frac{3e^2}{2r_0}$$

$$\left(\frac{4\pi r_0^3}{3}\right) = -\frac{e}{\rho}$$

$$U_c^{in} = -\frac{3\cancel{e^2}}{\cancel{2}r_0} \qquad 1 \text{ Ry}$$

$$\frac{\cancel{e^2}}{\cancel{2}a_H}$$

$$U_c^{in} = -\frac{3}{r_s} \quad \text{Rydberg.}$$

c) Coulomb self-energy

$$U_c^{self} = \rho^2 \int_0^{r_0} dr \left(\frac{4\pi r^3}{3}\right) \frac{(4\pi r^2)}{r} = \frac{3e^2}{5r_0}.$$

$$U_c^{self} = \frac{\frac{3\cancel{e^2}}{5r_0}}{\frac{\cancel{e^2}}{2a_H}} = \frac{6}{5r_s} \quad \text{Rydbergs.}$$

d) $$U_c^{ion} + U_c^{self} = \frac{-1.80}{r_s}.$$

Sum of Coulomb and kinetic energies is

$$U_{binding} = \frac{-1.80}{r_s} + \frac{2.21}{r_s^2}.$$

Minimum when

$$\frac{1.80}{r_s^2} = \frac{4.42}{r_s^3} \Rightarrow r_s = \frac{4.42}{1.8} = 2.45$$

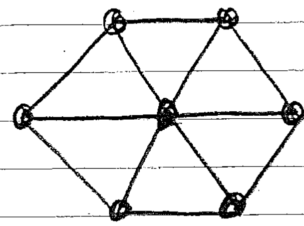
$$U_{binding}(r_s = 2.45) < 1 \text{ Rydberg}$$

($\sim .4$ Rydberg)

$\Downarrow$

Separated H atoms are more stable.

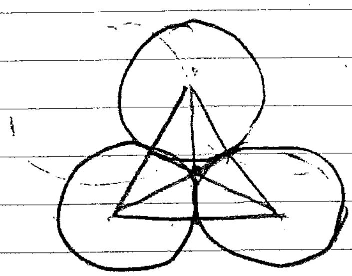
5. Let us represent the centers of the atoms (spheres w/ $r=a$) as points. Then a bottom layer hexagonal plaquette looks like



where we note that all the triangles are equilateral

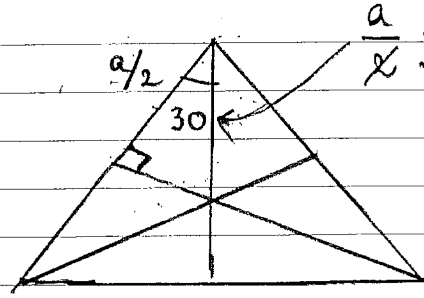
$$hcp = A\,B\,A\,B\ldots$$

The spheres of the second layer of an hcp structure are placed so that each is equidistant from the three neighboring triangular vertices (associated w/ the A layer.

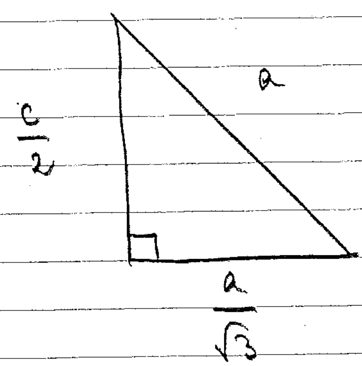


$\Rightarrow$

$$\frac{a}{\cancel{2}}\frac{\cancel{2}}{\sqrt{3}} = \frac{a}{\sqrt{3}}$$



In order to solve for c, we study the right triangle



$$\left(\frac{c}{2}\right)^2 + \frac{a^2}{3} = a^2$$

$$\left(\frac{c}{2}\right)^2 = \frac{2}{3}\, a^2$$

$$\left(\frac{c}{a}\right)^2 = \frac{8}{3} \Rightarrow \frac{c}{a} = \sqrt{\frac{8}{3}}$$

$$\frac{c}{a} = 1.633.$$

6. In order to determine the x- y- intercepts of these planes, we must invert the indices (thus running the Miller index prescription backwards)

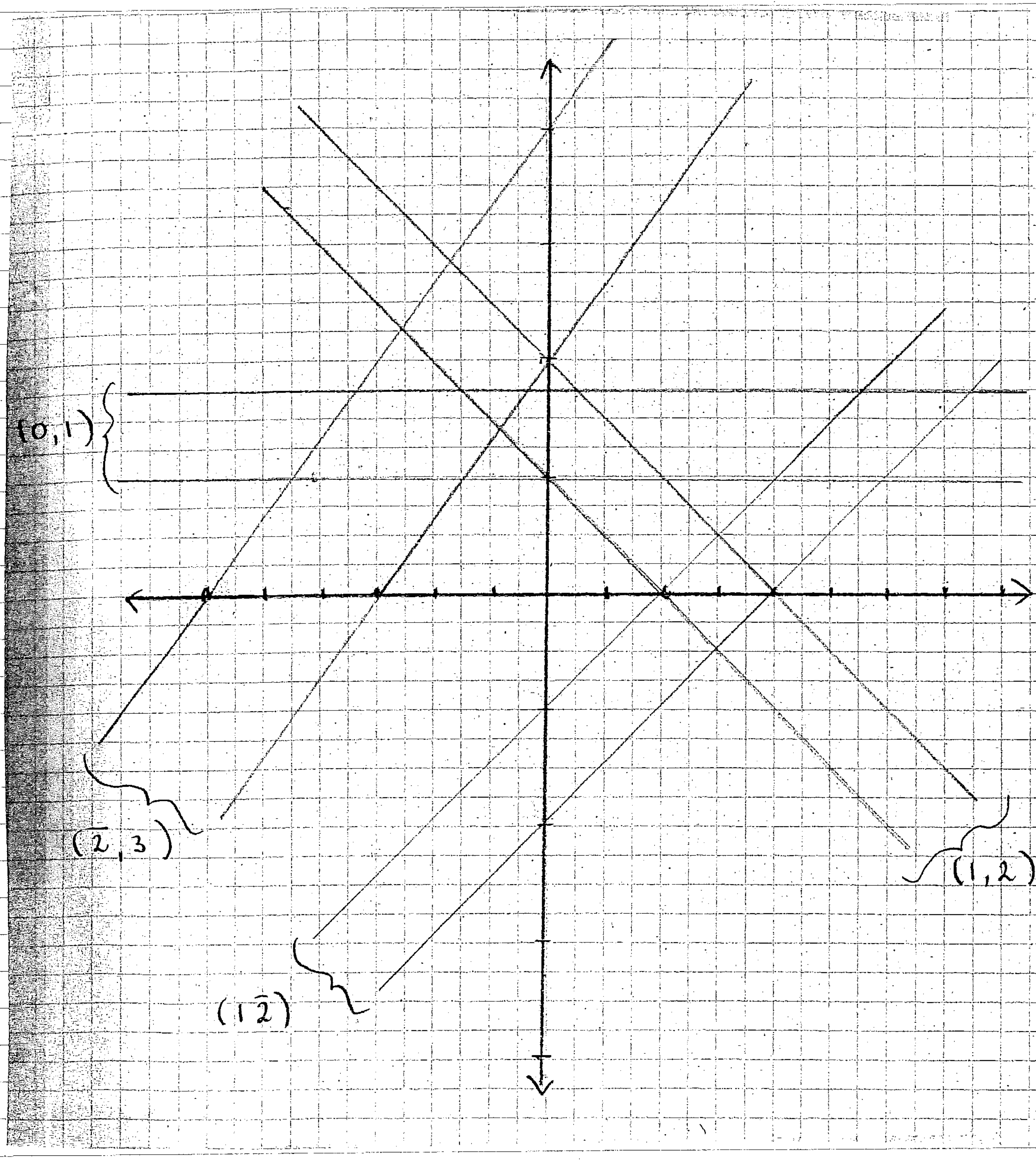
$(0\ 1) \rightarrow (1\ 0)$

$(1\ 2) \rightarrow \left(1\ \frac{1}{2}\right) \rightarrow (2\ 1)$

$(\bar{2}\ 3) \rightarrow \left(\frac{\bar{1}}{2}\ \frac{1}{3}\right) \rightarrow (\bar{3}\ 2)$

$(1\ \bar{2}) \rightarrow \left(1\ \frac{\bar{1}}{2}\right) \rightarrow (2\ \bar{1})$

The planes are displayed for a rectangular lattice $(a_2 = 2a_1)$ on the next page.


(0,1)
(2̄,3)
(1,2)
(1 2̄)

7. Quasicrystals are solids whose constituent atoms are arranged in neither periodic nor random structure. Diffraction from quasicrystals yields sharp spots despite the absence of translational symmetry. The constituents of quasicrystals are arranged in non-repeating structures that obey specific tiling rules.

8. The diffraction patterns of quasicrystalline materials displayed underlying "forbidden symmetries" that are known to be incompatible w/ space-filling structures. At the time of the discovery of these quasicrystalline materials it was believed that there exist two types of solid: a (periodic) crystal and a (random) glass. Furthermore it was believed that the presence of sharp spots in a diffraction pattern was indicative of underlying periodic order, which could not occur for structures with "forbidden" symmetries. Finally it was not clear

how a quasi-regular quasicrystal could develop using "local rules" but this was shown mathematically after a few years.

9. Diffraction Patterns of a Crystal and a Quasicrystal

(a) Similarities

Sharp spots

Patterns indicate some similar rotational symmetries (2- and 4-fold)

(b) Differences.

Quasicrystalline patterns display rotational symmetries (e.g. 5-fold) forbidden for crystalline materials

10. (a) Conductivity

The conductivity of a quasicrystalline material is less than its crystalline counterpart

(b) Hardness

A quasicrystal is harder to deform than is its crystalline counterpart

11. Two possible applications of quasicrystals

(a) Low-Friction Coatings

Cookware; engine components

(b) Hardness

Possible replacement for industrial diamonds.

12. In principle an icosahedral glass should have broader diffraction peaks than a quasicrystal since the latter but not the former has positional order. However practically there are always random distortions that develop during growth, so that most quasicrystalline materials are not ideal. However signatures of stress-induced phason strain, a distortion of the structure obtained by rearranging cells, will distinguish them; for the icosahedral glass it will be isotropic whereas it will be highly anisotropic for the quasicrystal.