

Quantum Condensed Matter Physics

2009

Short Questions:

[1]

(a) The attractive A/r^6 term is due to van der Waals forces between the atoms (1 mark), and the repulsive B/r^{12} term is a model of the short range repulsion caused by the overlap of the electron orbitals of the two atoms as the two atoms approach each other. (1.5 marks)

Van der Waals forces arise because the zero point motion/fluctuations of the electrons within an atom mean that the atom has an instantaneous electrostatic dipole moment, p_1 , which gives rise to an electric field around it of strength $E(r) \propto p_1/r^3$. If the neighbouring atom has a polarisability α , then this will induce a dipole of strength $p_2 = \alpha E(r) \propto \alpha p_1/r^3$. Since the energy of a dipole moment in an electric field is $-p \cdot E$, then the interaction potential produced by this means has an instantaneous value $\propto E \cdot \alpha p_1/r^3$ i.e. $\propto \alpha p_1^2/r^6$ averaging over time gives:

$$U_{\text{vdW}} \propto \alpha \langle p_1^2 \rangle / r^6 \text{ and since the average is over } p_1^2 \text{ it will be positive. (1.5 marks)}$$

(b) In many ways the electrons within a metal behave as if they could move freely through the structure, and indeed if one takes account of the fact that they are Fermions which restricts the electrons that have states into which they can move to those within roughly $k_B T$ of the Fermi level, quite a good model of the electrons within a conductor is obtained. However, as the electrons move, they do feel the effect of the periodic potential of the lattice, which affects the dispersion relation (E v. k) of the electrons. This influence may be included in the free electron model by replacing the real mass of the electron with an effective mass. (2 marks)

At the bottom of a band, the dispersion relation may be approximated as quadratic i.e.

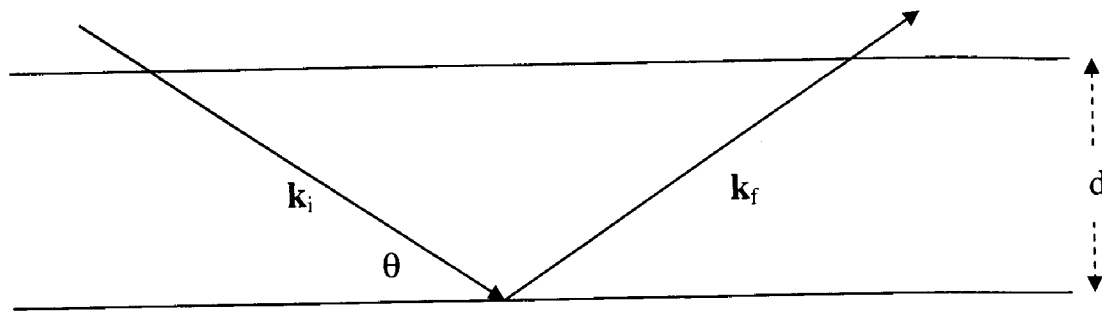
$$E(k) = \frac{1}{2} \frac{d^2 E}{dk^2} \bigg|_{k=0} k^2 \text{ (1 mark),. The free electron dispersion relation } (E = \frac{\hbar^2 k^2}{2m}) \text{ can be made to}$$

fit the actual dispersion relation by replacing the mass by an effective mass m^* so that

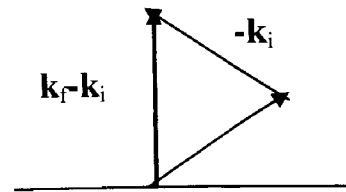
$$E = \frac{\hbar^2 k^2}{2m^*} = \frac{1}{2} \frac{d^2 E}{dk^2} \bigg|_{k=0} k^2 \text{ i.e. } m^* = \hbar^2 / \frac{d^2 E}{dk^2} \bigg|_{k=0}.$$

$$\text{Here } \frac{d^2 E}{dk^2} \bigg|_{k=0} = \hbar^2 / a^2 \text{ and so the effective mass is } m^* = \hbar^2 / a^2 A \text{ (1 mark).}$$

(c)



(Diagram 1mark) Firstly, consider direction of $\mathbf{k}_f - \mathbf{k}_i$:
 - clearly perpendicular to planes of atoms, and so parallel to lattice vector (\mathbf{G}_1) associated with these planes.
(1mark)



Magnitude of $\mathbf{k}_f - \mathbf{k}_i$ is $2k_i \sin \theta$ since $k_f = k_i$

Bragg condition gives:

$$2d \sin \theta = n\lambda$$

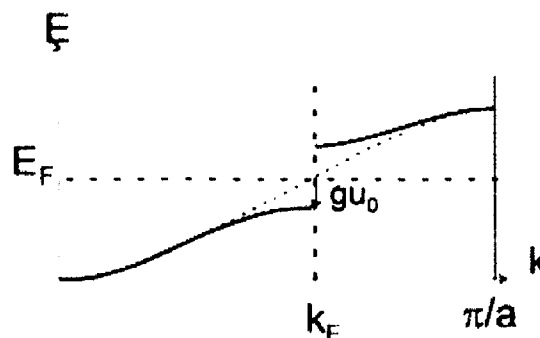
$$\Rightarrow 2 \cdot \frac{2\pi}{\lambda} \sin \theta = n \cdot \frac{2\pi}{d} = nG_1$$

$$\Rightarrow |\mathbf{k}_f - \mathbf{k}_i| = nG_1$$

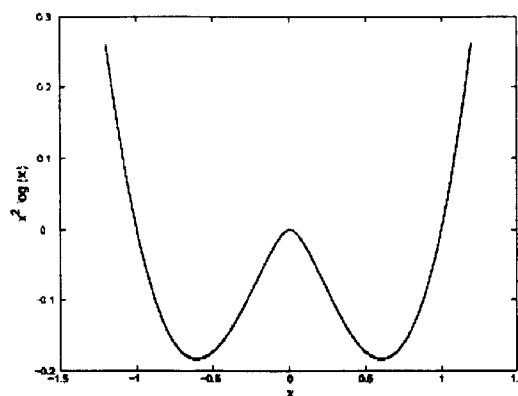
So magnitude of $\mathbf{k}_f - \mathbf{k}_i$ is that of a lattice vector since $n\mathbf{G}_1$ is also a lattice vector. **(2marks)**

[2] The answers to these section 2 questions reflects the most that one can expect, but really one is giving **1 mark per sensible point**, and full marks can be obtained with less than these full answers.

(a) - If a spontaneous fluctuation of a the lattice produces a periodic potential of the lattice of wave vector Q and if Q happens to be equal to the Fermi wave vector, then the periodic distortion of the lattice will induce a gap at the Fermi level, causing the energy of the occupied states (particularly those near the Fermi level) to drop, (diagram) hence lowering the energy of the system.



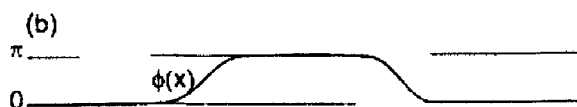
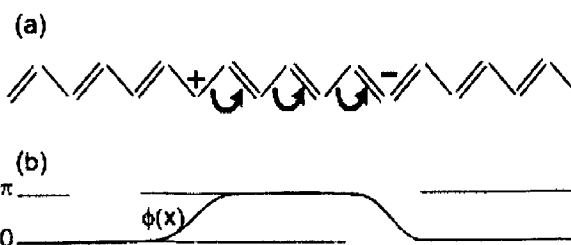
-For a 1d system this works perfectly, whereas for a higher dimensional system, only part of the Fermi surface aligns with Q and the size of the effect depends on the fraction of the Fermi surface that is parallel to another part of the Fermi surface perpendicular to the direction of interest in the crystal. This is associated with oscillations in the charge density, with the same wavevector. The energy of the electrons is change by an amount $E_{\text{electronic}} = A(u_0/a)^2 \ln |u_0/a|$ where u_0 is the ampliude of the periodic distortion of the lattice. The elastic energy associated with this distortion is given by: $E_{\text{elastic}} = K(u_0/a)^2$ since the sum of these always has a minimum at finite u_0 (see sketch form of $x^2 \ln x$), one will always get a CDW in 1D, i.e. the energy reduction obtained by dropping the energy of the states just below the Fermi level compensates for the elastic energy required to distort the lattice at a wavelength Q . The formation of this distortion is know as a Peierls Transition.



- Observation – can get an electron/xray/neutron diffraction pattern from them, and one can see them as a softening of phonons at k_F .

- Classic case is polyacetylene. The $-C-C-C$ change has on average a bond order of 1.5, but this splits into double and single bonds: $-C=C-C=C-$

- Again, considereing polyacetylene – can get domains of CDW since there are two ways the distortion can lock into the underlying lattice: - the phase ϕ between the CDW and the lattice can either be 0 or π .



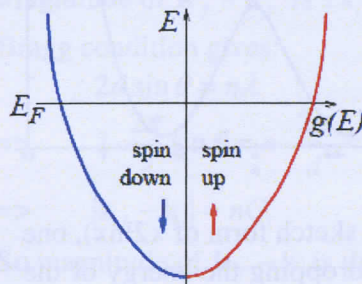
- By introducing boundaries, ('solitions') entropy up, hence thermodynamically stable, though they may not be well ordered – a type of glassy state

- To go from one lock in to another need to compress (charge up, net negative e) or rarify the CDW (less charge, hole, positive charge). An applied electric field will move these solitons giving conduction, but this can be highly non linear as the solitons can be pinned by defects, requiring a certain field before they start to move.

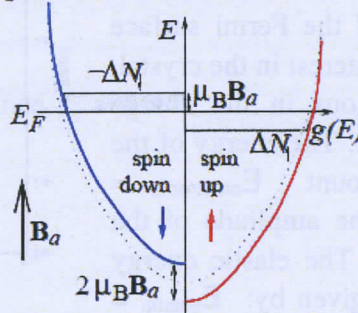
(b) Marking note: There is a lot that they can write on this one. But, they do need to explain the origin of paramagnetism, the fact that magnetic interactions alone cannot produce ferromagnetism at reasonable temperatures, and explain the exchange interactions that do give rise to ferromagnetic ordering. In each section of the answer the full answer as per their notes is given, however one is actually expecting a cut down version of a lot of this.

First one needs to understand origin of paramagnetism. In metals one either has two effects: For mobile electrons – use Pauli paramagnetism idea:

- Central quantity: **density of states** at E_F , $g(E_F)$.
- Magnetic **field off**: Up and down spins have **equal energy**.



Magnetisation in finite field:



- Spin-up electrons get more:
 $\Delta N_{\uparrow} = \frac{1}{2} \mu_B B g(E_F)$
- Spin-down electrons get fewer:
 $\Delta N_{\downarrow} = -\frac{1}{2} \mu_B B g(E_F)$

- Total no. of electrons (per unit volume): $N = N_{\uparrow} + N_{\downarrow}$
- Magnetisation: $M = \mu_B (N_{\uparrow} - N_{\downarrow})$

- Resulting **magnetisation**:
 $M = \mu_B^2 g(E_F) B$
 $= \mu_B^2 g(E_F) \mu_0 H$
- Paramagnetic metal:
Pauli susceptibility

$$\chi_P = \frac{dM}{dH} = \mu_0 \mu_B^2 g(E_F)$$

For the case of, for example, localized f electrons which cannot move freely through the crystal, can simply work out the mean dipole moment. If one takes for example a state where one had a single unpaired electron with dipole moment μ_B then the mean dipole moment would be:

$$\bar{\mu} = \mu_B \cdot (\text{Prob moment up} - \text{prob moment down}) = \mu_B \frac{\exp(\mu_B B / k_B T) - \exp(-\mu_B B / k_B T)}{\exp(\mu_B B / k_B T) + \exp(-\mu_B B / k_B T)}$$

$$= \mu_B \tanh(\mu_B B / k_B T)$$

For $\mu_B B / k_B T < 1$ $\tanh(\mu_B B / k_B T) \approx \mu_B B / k_B T$ and since $M = n\bar{\mu}$

$$\chi = \frac{M}{H} = \frac{M}{B / \mu_0} = \frac{n \mu_B^2 B}{k_B T} \text{ s}$$

And the material is again paramagnetic.

The magnetic interaction between spin or orbital magnetic moments is very small – far too small to produce ordering (ferromagnetism) at all but the very lowest temperatures. Before advent of quantum mechanics, in order to explain ferromagnetism Weiss proposed a molecular field proportional to the magnetization ($B_{mol} = \mu_0 \lambda M$) which caused the ordering of ferromagnetism. *i.e.* the total field experienced by a magnetic moment is:

$$B_{eff} = B_{ext} + \mu_0 \lambda M$$

The question is what could give rise to this molecular field. Electrons are Fermions so the total wavefunction must be asymmetric. Consider just two electrons. If the electrons have the same spin state (i.e. spins aligned) then the spin part of the wavefunction is symmetric, which forces the spatial part of the wavefunction to be anti-symmetric. In an antisymmetric wavefunction the chance of both electrons being in the same place is zero, i.e. they tend to avoid each other, and the electrostatic energy is reduced, giving the state with the spins of the two electrons parallel a low energy. This is the origin of Hund's rules for deciding which is the lowest energy configuration of electrons in an atom, but also will give tend to align the spins of two electrons if their wavefunctions overlap

In the Stoner-Hubbard model, to model the effect of this 'exchange interaction' which reduces the energy if the spins are parallel, a 'mean field' approach is used – i.e. the energy change of a spin up electron in the presence of a density of n_{\downarrow} spin down electrons is given by Un_{\downarrow} . The change in the number of spin up and spin down electrons is then:

$$\Delta n_{\uparrow} = [Un_{\downarrow} + \mu_B B] \frac{g(E_F)}{2}, \quad \Delta n_{\downarrow} = -[Un_{\uparrow} + \mu_B B] \frac{g(E_F)}{2}$$

and:

$$n_{\uparrow} - n_{\downarrow} = [U(n_{\uparrow} - n_{\downarrow}) + 2\mu_B B] \frac{g(E_F)}{2}$$

Since the magnetization is $M = \mu_B (n_{\uparrow} - n_{\downarrow})$ and $\chi = \frac{M}{H} = \frac{M}{B/\mu_0} = \frac{\mu_0 \mu_B^2 g(E_F)}{1 - \frac{Ug(E_F)}{2}}$ which will

diverge if U is big enough - i.e. the Stoner criterion is satisfied $\frac{Ug(E_F)}{2} > 1$, giving ferromagnetism.

Rare earth metals have partially occupied f orbitals. These electrons are not free to move, and indeed even within a tight binding model, the band width is very small because the f orbitals do not overlap on neighbouring atoms. The spins of f orbital electrons on neighboring atoms can still be aligned, but the localized f electrons interaction with mobile s, p, d , which in turn interact with the f electrons on the neighbouring atoms.

$$\chi = \frac{M}{H} = \frac{M}{B/\mu_0} = \frac{\mu_0 \mu_B^2 g(E_F)}{1 - \frac{Ug(E_F)}{2}}$$

Using a Weiss like formalism: $B_{eff} = B_{ext} + \mu_0 \lambda M$ and as an example, taking an atom with one unpaired electron, which can either be aligned (energy $-\mu_B B_{eff}$) or down (energy $\mu_B B_{eff}$) with respect to the effective field. The mean magnetic moment in the direction of the field will be:

$$\bar{\mu} = \mu_B \frac{\exp(\mu_B B_{eff} / k_B T) - \exp(-\mu_B B_{eff} / k_B T)}{\exp(\mu_B B_{eff} / k_B T) + \exp(-\mu_B B_{eff} / k_B T)} = \mu_B \tanh(\mu_B B_{eff} / k_B T)$$

and for a number density n , the magnetization $M = n\bar{\mu} = n\mu_B \tanh(\mu_B B_{eff} / k_B T)$. For no external field $B_{eff} = \mu_0 \lambda M$ and $M = n\bar{\mu} = n\mu_B \tanh(\mu_B \mu_0 \lambda M / k_B T)$. To solve this graphically, rearrange:

$$\frac{M}{n\mu_B} = \tanh(\mu_B \mu_0 \lambda M / k_B T)$$

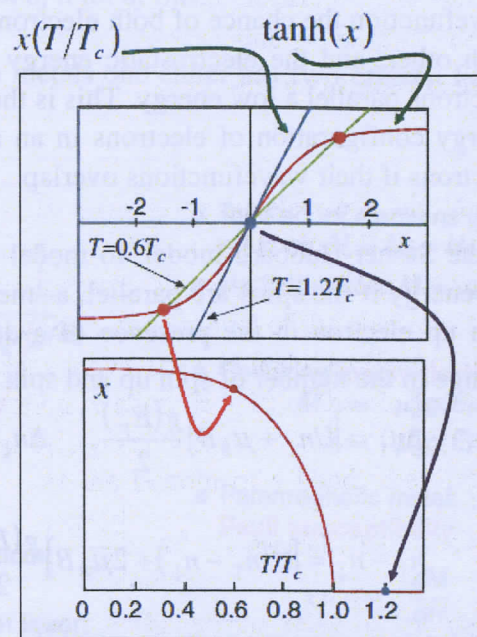
Using: $x = \mu_B \mu_0 \lambda M / k_B T$, then

$$\frac{M}{n\mu_B} = \frac{\mu_B \mu_0 \lambda M}{k_B T} \cdot \frac{k_B T}{\mu_B \mu_0 \lambda n\mu_B} = x \frac{T}{T_c}$$

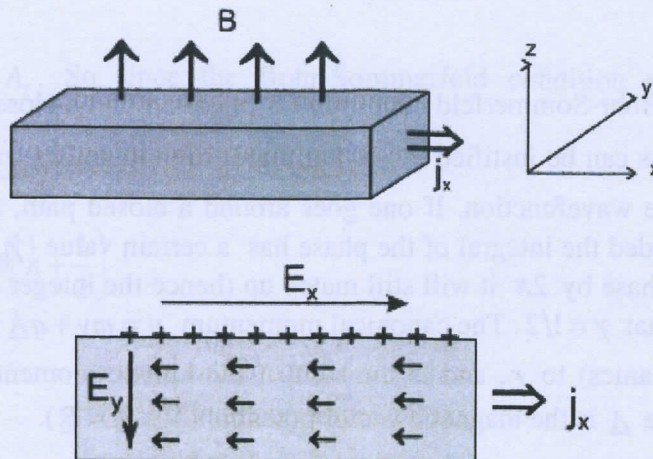
where $T_c = \frac{n\mu_B^2 \mu_0 \lambda}{k_B}$ and we are trying to solve:

$$x \frac{T}{T_c} = \tanh(x)$$

which we can do graphically by looking for the intersection of the lines $x \frac{T}{T_c}$ and $\tanh(x)$. For $T > T_c$ the lines do not intersect, and the system is not ferromagnetic but for $T < T_c$ magnetization at finite fields exists.



(c) If a B field (z direction – see diagram) is applied perpendicular to a conductor carrying a current (x direction), the Lorentz force will push the charge carriers perpendicular to both (y direction), causing charge to build up on the sides of the conductor which produces a E field that prevents further movement of charge in y the direction. This is the Hall voltage, and the whole process is called the Hall effect. The net force on a carrier is given by:



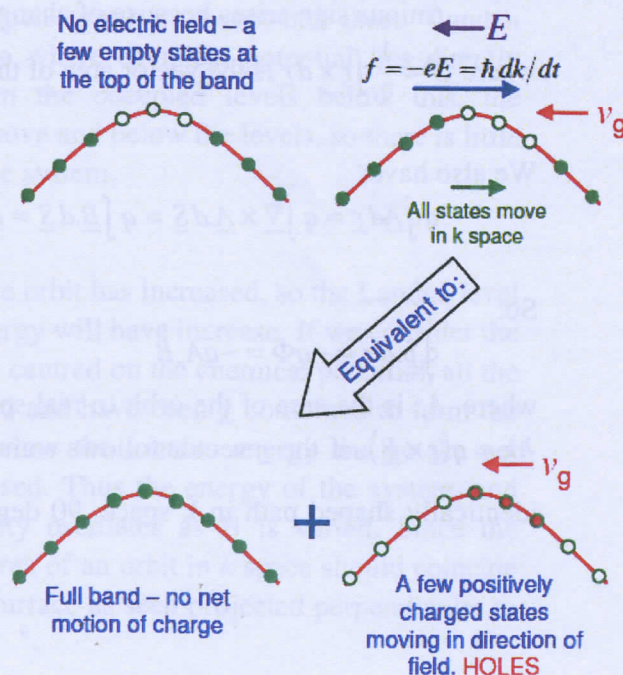
$$\mathbf{F} = q(\mathbf{E} + \mathbf{v} \times \mathbf{B}) = q(\mathbf{E} + \mathbf{v}_{drift} \times \mathbf{B}) + q\mathbf{v}_c \times \mathbf{B}$$

Where the velocity \mathbf{v} can be decomposed into a drift velocity \mathbf{v}_{drift} (in the x direction) such that the Lorentz force due to it counterbalances the E field in the y direction, i.e. $\mathbf{E} + \mathbf{v}_{drift} \times \mathbf{B} = 0$ and a remaining velocity \mathbf{v}_c due to the electron tending to perform cyclotron orbits in the field. Both of these velocities are interrupted by collisions of the electrons with phonons or defects in the solid – the drift velocity is maintained by a field along the conductor.

$\mathbf{E} + \mathbf{v}_{drift} \times \mathbf{B} = 0$ implies that (for conventionally positive charge flowing) $E_y - v_{drift} B_z = 0$. For a carrier density n , the current density is given by $nq\mathbf{v}_{drift}$, so: $E_y = v_{drift} B_z = \frac{j_x}{nq} B_z$. The Hall

coefficient is defined by: $R_H = \frac{E_y}{j_x B_z} = \frac{1}{nq}$. In the

free electron model, the current is carried by a drift velocity of all the electrons in the metal, and so n is the free electron density, and q is negative, so the R_H is negative. For many metals (e.g. alkali metals, typical transition metals – e.g. copper, or for example aluminium) this works well, because these metals can be understood in terms of the free electron model, since the Fermi level does not fall in a band gap. If, however, as is the case for some divalent metals such as Be and Cd, and indeed for p-doped semiconductors, one gets a positive Hall coefficient, implying positive charge carriers. This arises because in these materials we have a nearly full band, with a few empty states at the top. Now need some explanation of hole conduction – see diagram.



B3:

The Bohr-Sommerfeld condition for phase around a closed orbit: $\oint \underline{p} \cdot d\underline{r} = 2\pi\hbar(n + \gamma)$. The form of this can be justified by saying that if the integral of $\underline{p} \cdot d\underline{r}/\hbar$ along a path is the phase change of the wavefunction. If one goes around a closed path, then if you find that the path closes up provided the integral of the phase has a certain value (γ) then if you increase the path integral of the phase by 2π it will still match up (hence the integer n in the equation). For electrons it turns out that $\gamma = 1/2$. The canonical momentum $\underline{p} = m\underline{v} + q\underline{A}$ is the conjugate variable (in Lagrangian mechanics) to \underline{r} , and is the sum of the kinetic momentum $m\underline{v}$ and the field momentum $q\underline{A}$, where \underline{A} is the magnetic vector potential ($\nabla \times \underline{A} = \underline{B}$).

The Lorenz force on a moving charged particle in magnetic field gives an acceleration to the particle:

$$m\dot{\underline{v}} = q(\dot{\underline{v}} \times \underline{B})$$

This can be integrated w.r.t to give:

$$m\underline{v} = q(\underline{r} \times \underline{B}) + \underline{v}_0$$

Where \underline{v}_0 is a constant. Setting $\underline{v}_0 = 0$ gives orbits in a plane perpendicular to \underline{B} with \underline{r} measured for the centre of the orbits. The integral $\oint \underline{p} \cdot d\underline{r}$ now becomes:

$$\oint \underline{p} \cdot d\underline{r} = \oint (m\underline{v} + q\underline{A}) \cdot d\underline{r} = \oint q(\underline{r} \times \underline{B}) \cdot d\underline{r} + \oint q\underline{A} \cdot d\underline{r}$$

Now

$$q \oint (\underline{r} \times \underline{B}) \cdot d\underline{r} = -q\underline{B} \cdot \oint \underline{r} \times d\underline{r} = -2q\underline{B} \cdot \underline{S} = -2q\Phi$$

(minus sign arises because of change of order of scalar triple product)

where $\underline{S} = \frac{1}{2} \oint \underline{r} \times d\underline{r}$ is the vector area of the loop, and Φ is the magnetic flux linked to the loop.

We also have:

$$q \oint \underline{A} \cdot d\underline{r} = q \int \nabla \times \underline{A} \cdot d\underline{S} = q \int \underline{B} \cdot d\underline{S} = q\Phi$$

So:

$$\oint \underline{p} \cdot d\underline{r} = -q\Phi = -qA_r B$$

where A_r is the area of the orbit in real space perpendicular to \underline{B} . Given that $m\underline{v} = q(\underline{r} \times \underline{B})$, i.e. $\hbar \underline{k} = q(\underline{r} \times \underline{B})$, if the \underline{r} vector follows some closed path in real space the \underline{k} vector will follow an identically shaped path in k space, 90 degrees rotated scaled in size by $\frac{qB}{\hbar}$, so the area of the

loop in k space, A_k will be $\left(\frac{qB}{\hbar}\right)^2 A_r$. So since the Bohr-Sommerfeld condition gives

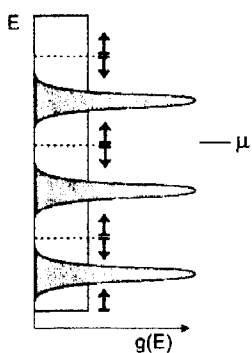
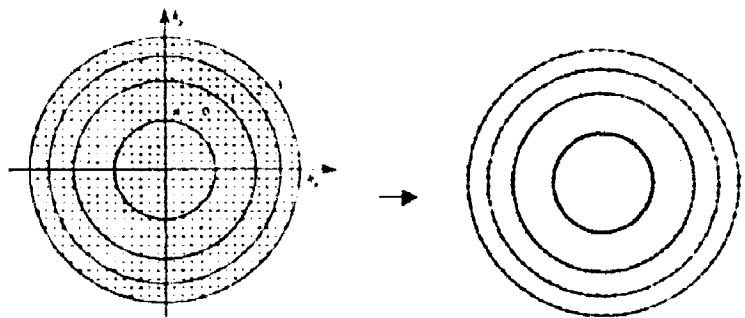
$\oint \underline{p} \cdot d\underline{r} = -q\Phi = -qA, B = 2\pi\hbar\left(n + \frac{1}{2}\right)$ we have:

$$qA, B = q\left(\frac{\hbar}{qB}\right)^2 A_k B = 2\pi\hbar\left(n + \frac{1}{2}\right)$$

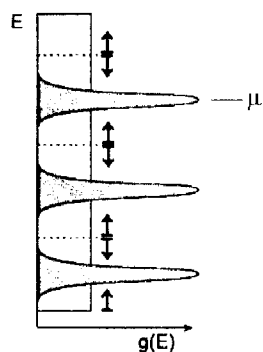
and:

$$A_k = B \frac{2\pi q}{\hbar} \left(n + \frac{1}{2}\right)$$

Without a B field the permitted k states are uniformly distributed in k space (left hand side of diagram below). With the B field on, and looking down the B axis in k space, one sees then that the k must lie on an orbit with an area corresponding to a particular value of n , so all the states that were distributed between these orbits will have been swept into the nearest permitted orbit.



All the states swept into one orbit have the same energy, though this energy is broadened by disorder (or finite lifetime of an electrons path as it goes around an orbit before being scattered by a defect, or a phonon). In the diagram (left) the original states (pale grey) are swept into these 'Landau levels' (dark grey). Consider case where chemical potential lies directly between two Landau levels – in the occupied levels below this, the electrons have come from states above and below the levels, so there is little net change in the total energy of the system.



At a higher B field the area of the orbit has increased, so the Landau level below the chemical potential energy will have increased. If we consider the case where it has increased to be centred on the chemical potential, all the original states that were occupied and have been χ combined to form the new level were of an energy below the Landau energy and so the net energy of the system has increased. Thus the energy of the system, and hence the magnetic susceptibility oscillates as B is varied. Since the condition of interest is that the area of an orbit in k space should coincide with the area inside the Fermi surface as seen projected perpendicular to the B field, $A_k = A_F$ we have:

$$A_F = B \frac{2\pi q}{h} \left(n + \frac{1}{2} \right)$$

i.e. the B field at which this occurs is given by:

$$\frac{1}{B} = \frac{1}{A_F} \frac{2\pi q}{h} \left(n + \frac{1}{2} \right)$$

So, if the orbits close up for a particular value of n , this matching of areas will again when n changes by 1, i.e. when the change in $\frac{1}{B}$, written as $\Delta\left(\frac{1}{B}\right)$ is given by $\Delta\left(\frac{1}{B}\right) = \frac{1}{A_F} \frac{2\pi q}{h}$. and

$$A_k = A_F = \frac{2\pi q}{h} \frac{1}{\Delta\left(\frac{1}{B}\right)} NA$$

Whilst any closed orbit will give rise to oscillations in χ , the only ones observed in a measurement of χ as a function of B will be those where there are lots of orbits that have the same area. This occurs for so called external orbits, where the orbit lies at some extreme point of the Fermi surface as seen in its projection perpendicular to B.

[11 marks] (marking note – clearly the candidates can write this more succinctly in not e form. Key points that must be present for full marks are Born-Sommerfeld, canonical momentum, derivation, understanding that states are reformed on rings, understanding how energy will vary as B varies, hence χ oscillations.)

The $|d_{xy}\rangle$ orbitals only hybridize with neighbours in the xy plane, giving a 2D band structure – i.e. one that does not vary with z. We are told this is a cylinder parallel to the z axis, so A_k corresponds to the cross sectional area of the cylinder. Putting the numbers into the expression for the area A_k we obtain

$$A_k = \frac{2\pi \cdot 1.602e-19}{1.05459e-34} \cdot 1.8e4 = 1.72 \text{ \AA}^2 \quad \text{[2 marks]}$$

Since: $A_k = \pi k_F^2$ we have $k_F = 0.74 \text{ \AA}^{-1}$. [1 marks]

If we have a 2d sample of side length Na where a is the unit cell length, then the k states will be separated by $\frac{2\pi}{Na}$ in k space, having an area each of $\left(\frac{2\pi}{Na}\right)^2$. The band has 4/3 electrons per unit cell in it, so the number of occupied states inside the Fermi circle is given by:

$$\frac{4}{3} N^2 = 2 \frac{\pi k_F^2}{\left(\frac{2\pi}{Na}\right)^2}$$

(the 2 is because of the spin degeneracy of each states). Since $\pi k_F^2 = A_k$ we have:

$$A_F = \frac{2}{3} \left(\frac{2\pi}{a} \right)^2 \quad \text{[2 marks]}$$

Hence: $a = 2\pi \sqrt{\frac{2}{3A_F}} = 3.91 \text{ \AA}$

[1 marks]

The $|d_{xz}\rangle$ orbitals only hybridize with neighbouring $|d_{xz}\rangle$ orbitals in the x direction – i.e. they give rise to a 1D band structure. [1 mark] In the tight binding model of a band structure with nearest neighbour interactions only and an overlap integral between neighbouring atoms of t the energy of the states in the band is given as a function of the k vector by:

$$E(k) = E_0 + t \cos(ka)$$

In this case we have a three dimensional wavevector, but the energy is a function of its x component only so:

$$E(\underline{k}) = E_0 + t \cos(k_x a)$$

[1 mark]

In 3D these one D bands have an energy depending only on k_x , so the Fermi surface for the band formed by the $|d_{xz}\rangle$ orbitals (the A Fermi sheet) will be 2 planes normal to the x direction at perpendicular distances of $\pm k_F$ from the plane $x = 0$, and similarly for the $|d_{yz}\rangle$ orbitals (the B Fermi sheet) but rotated 90 degrees about the z axis.

Considering the band formed by the $|d_{xz}\rangle$ orbitals we the occupied states lie between $\pm k_F$ along the x axis, but fill the Brillouin zone in the y direction – thus taking an area of $2k_F \cdot 2\frac{\pi}{a}$ in k space

As previously the band has $4/3$ electrons per unit cell in it, so the number of occupied states inside the Fermi circle is given by:

$$\frac{4}{3} N^2 = 2 \frac{4k_F \frac{\pi}{a}}{(2\pi/Na)^2}$$

and we have:

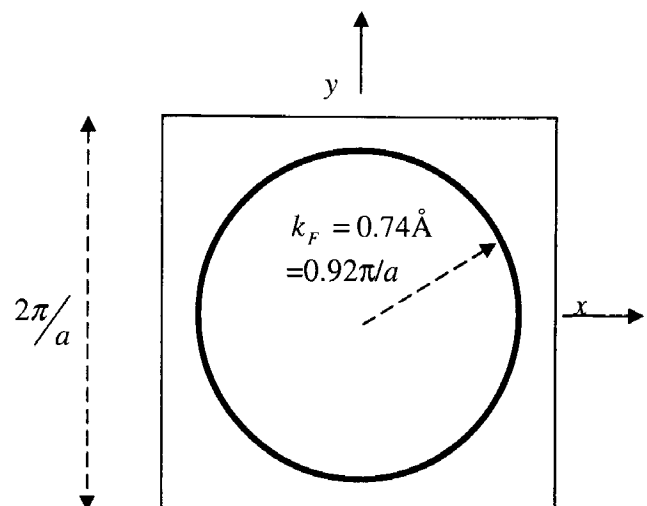
$$k_F = \frac{2}{3} \frac{\pi}{a} \quad [3 \text{ marks}]$$

Sketching: [3 marks]

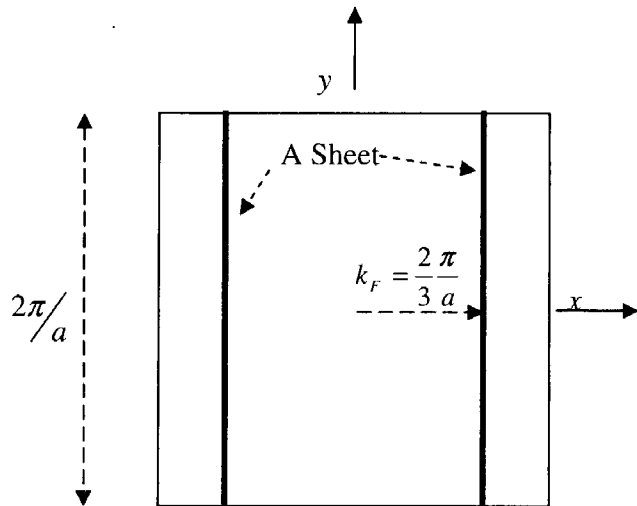
For the γ sheet looking down the z axis onto the xy plane – the cylinder is a circle radius $k_F = 0.74 \text{ \AA} = 0.92\pi/a$.

$$A_k = \pi k_F^2$$

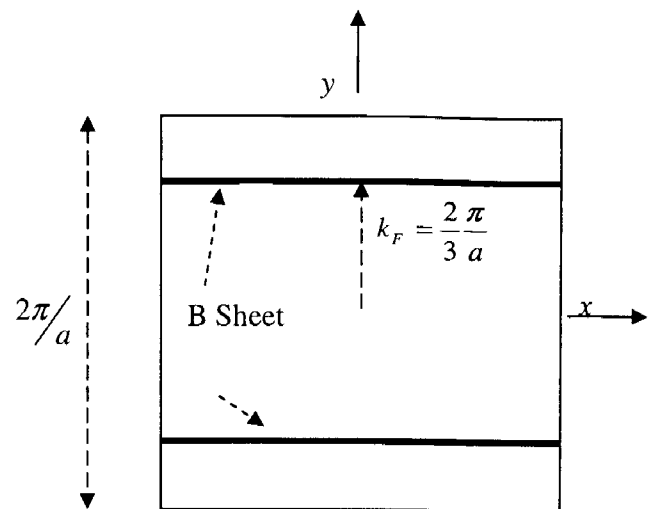
Giving $k_F = 0.74 \text{ \AA} = 0.92\pi/a$



A Fermi sheets:



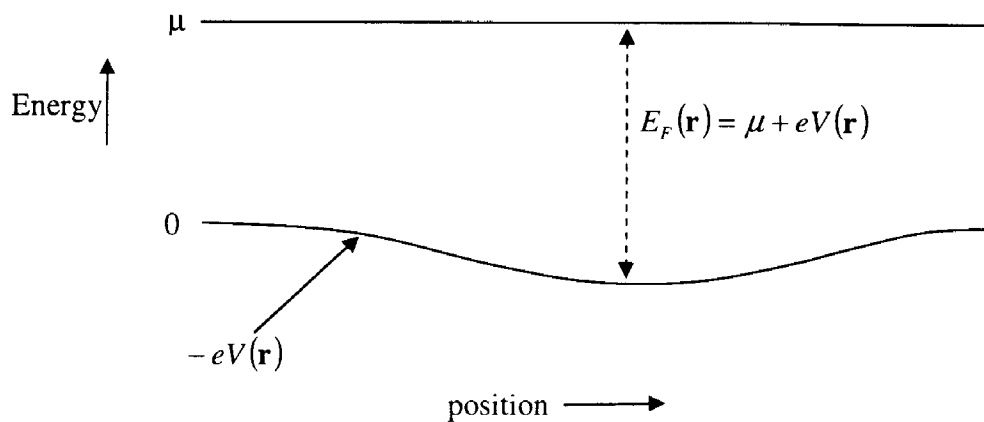
B Fermi Sheets



B4:

An electric field inside a conductor causes charge to move. In macroscopic electrostatics (where there is no long term electric current), the charge moves until the field inside the conductor is exactly cancelled out. Macroscopic electrostatics does not take account of the Pauli exclusion principle, which means that in the ground state a range of states will be occupied by the charge carriers, and these include a lot of kinetic energy. If you increase the charge density in response to an electric field in the conductor this kinetic energy will rise, and there is a trade off between reducing the energy stored in the electrostatic field and increasing the kinetic energy of the charge carriers, and so on the atomic scale the lowest energy state corresponds to only imperfect screening at short distances, whereas at large distances perfect screening is obtained – if there is an electric field at large distances the electrostatic energy diverges and it is energetically worth while for the system to move charge to screen it. **[4 marks]**

TF theory assumes an ‘independent particle approach’ in which the electrons move in a mean field given by the other electrons and the ion cores. The ion core potential is thus represented by a uniform positive background. It assumes that the potential changes only slowly over the length scale of the Fermi wavevector so that the kinetic energy of the electrons may be expressed in terms of a local Fermi Energy, derived from the free electron model. The zero of the local energy is offset by the electrostatic potential, so the local Fermi energy is given by $E_F(\mathbf{r}) = \mu + eV(\mathbf{r})$. (note e is the magnitude of the electronic charge)



[3 marks for approximations involved in TF theory, 2 marks for explaining equation]

$$\text{Since } E_F = \frac{\hbar^2}{2m} (3\pi^2 n)^{2/3} = \alpha n^{2/3}$$

$$\Rightarrow \frac{dE_F}{dn} = \frac{2}{3} \alpha n^{-1/3} = \frac{2}{3} \alpha n^{-1/3} \cdot \frac{n}{n} = \frac{2}{3} \frac{E_F}{n}$$

and for small changes:

$$\delta E_F = \frac{2}{3} \frac{E_{F0}}{n_0} \delta n$$

Now: $E_F(\mathbf{r}) = \mu + eV(\mathbf{r})$ and $\mu = E_{F0}(\mathbf{r})$ so for a small V :

$$E_F(\mathbf{r}) - E_{F0}(\mathbf{r}) = \delta E_F = eV(\mathbf{r}) = \frac{2}{3} \frac{E_{F0}}{n_0} \delta n = \frac{2}{3} \frac{E_{F0}}{n_0} [n(r) - n_0]$$

$$\Rightarrow [n(r) - n_0] = \frac{3}{2} \frac{n_0}{E_{F0}} eV(\mathbf{r})$$

(remember V is a positive number in the way this problem is set up)

The induced charge density is $\rho_{ind} = -e[n(r) - n_0]$ so:

$$\rho_{ind} = -\frac{3}{2} \frac{n_0}{E_{F0}} e^2 V(\mathbf{r})$$

Note, we are assuming that there is no induced charge density due to polarisation of the ion cores, but this approximation is within the TF theory since we are replacing the ion cores by a uniform positive background. **[6 marks]**

For a point charge located at $r = 0$, ρ_{free} is zero everywhere except at $r = 0$, so for $r \neq 0$ and substituting for ρ_{ind} gives:

$$\nabla^2 V = -\frac{1}{\epsilon_0} \rho_{ind} = \frac{1}{\epsilon_0} \cdot \frac{3}{2} \frac{n_0}{E_{F0}} e^2 V = \beta V \quad \text{where for convenience } \beta = \frac{3n_0 e^2}{2\epsilon_0 E_{F0}}$$

Substituting $V(r) \propto \frac{1}{r} \exp\left(-\frac{r}{\xi}\right)$ gives:

$$\begin{aligned} \Rightarrow \nabla^2 \left[\frac{1}{r} \exp\left(-\frac{r}{\xi}\right) \right] &= \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) \left[\frac{1}{r} \exp\left(-\frac{r}{\xi}\right) \right] \\ \Rightarrow &= \frac{1}{r} \frac{\partial}{\partial r} \left(r^2 \left[-\frac{1}{r^2} \exp\left(-\frac{r}{\xi}\right) - \frac{1}{r\xi} \exp\left(-\frac{r}{\xi}\right) \right] \right) \\ \Rightarrow &= \frac{1}{r} \frac{\partial}{\partial r} \left[-\exp\left(-\frac{r}{\xi}\right) \left(1 + \frac{r}{\xi} \right) \right] \\ \Rightarrow &= \frac{1}{r} \left[\frac{1}{\xi} \exp\left(-\frac{r}{\xi}\right) \left(1 + \frac{r}{\xi} \right) - \exp\left(-\frac{r}{\xi}\right) \left(\frac{1}{\xi} \right) \right] \\ \Rightarrow &= \frac{1}{\xi^2} \exp\left(-\frac{r}{\xi}\right) = \beta \exp\left(-\frac{r}{\xi}\right) \end{aligned}$$

$$\text{if } \xi = \frac{1}{\sqrt{\beta}} = \sqrt{\frac{2\epsilon_0 E_{F0}}{3n_0 e^2}} \quad \text{qed}$$

[5 marks]

For sodium $n_0 = 968 / (23.0e - 3 / 6.0223e23) = 2.534e28 \text{ m}^{-3}$, and

$$E_{F0} = \frac{\hbar^2}{2m} (3\pi^2 n_0)^{2/3} = \frac{(1.05459e-34)^2}{2 \times 9.1096e-31} (3\pi^2 2.534e28)^{2/3} = 5.040e-19 \text{ J}$$

$$\text{So: } \xi = \sqrt{\frac{2\epsilon_0 E_{F0}}{3n_0 e^2}} = \sqrt{\frac{2 \times 8.854e-12 \times 5.040e-19}{3 \times 2.534e28 \times 1.602e-19^2}} = 6.76e-11 \text{ m, i.e. } 0.68 \text{ \AA} \quad [1 \text{ mark}]$$

Since the wavelength corresponding to the Fermi wavevector is:

$$\lambda_F = \frac{2\pi}{k_F} = \frac{2\pi}{(3\pi^2 n_0)^{1/3}} = \frac{2\pi}{(3\pi^2 2.534e28)^{1/3}} = 6.91e-10 \text{ m, i.e. } 6.9 \text{ \AA}, \text{ the theory is well and}$$

truly being applied outside its limits (i.e. $\xi \gg \lambda_F$). Clearly the screening length is small – on the atomic scale, but the theory is being applied so far outside its limits that it is of questionable value, and one is back to ones first impression that the screening length must be of the order of the size of an atom, since the electrons around an atom screen the core by the time one is outside the atom, which is somewhat quicker than TF theory. [2 marks]

The remarkable thing about this observation is that the force constant for the 2 layer film is effectively the same as bulk sodium. Since the elastic properties of a nearly free electron metal such as Na are largely determined by the electrons, this shows that the electrons between the e layers of sodium behave as though they are in bulk sodium. This is consistent with the very short screening length – i.e. the surfaces of the 2 atomic layer thick film are too far away to have much influence on the electrons between the layers. [examiners note: these measurements are described in Benedek *et. al.* Phys. Rev. Lett. **69**, 2951 (1992)] [2 marks]