

## Level 3 Condensed Matter Physics- Part II

### Examples Class 1 Answers

(1) (i) The Bloch wavefunction is given by  $\psi_{n\mathbf{k}}(\mathbf{r}) = u_{n\mathbf{k}}(\mathbf{r})\exp(i\mathbf{k}\cdot\mathbf{r})$ , where  $u_{n\mathbf{k}}(\mathbf{r})$  has the periodicity of the crystal (i.e.  $u_{n\mathbf{k}}(\mathbf{r}+\mathbf{T}) = u_{n\mathbf{k}}(\mathbf{r})$  for any lattice translation vector  $\mathbf{T}$ ).  $\mathbf{k}$  is the wavevector and  $n$  the band index. Bloch functions differ from the plane wave, free electron solution by the additional term  $u_{n\mathbf{k}}(\mathbf{r})$ . This ensures that the electron *intensity* has the same periodicity as the crystal (i.e.  $|\psi_{n\mathbf{k}}(\mathbf{r}+\mathbf{T})|^2 = |\psi_{n\mathbf{k}}(\mathbf{r})|^2$ ). Note that  $|\psi|^2$  is a measurable quantity, but not the wavefunction  $\psi$ .

(ii) The momentum operator is given by  $\mathbf{p} = -i\hbar\nabla$ . Applying this to a Bloch function:

$$-i\hbar\nabla[u_{n\mathbf{k}}(\mathbf{r})e^{i\mathbf{k}\cdot\mathbf{r}}] = -i\hbar e^{i\mathbf{k}\cdot\mathbf{r}}\nabla u_{n\mathbf{k}} + \hbar\mathbf{k}\psi_{n\mathbf{k}}(\mathbf{r}) \neq \mathbf{p}\psi_{n\mathbf{k}}(\mathbf{r})$$

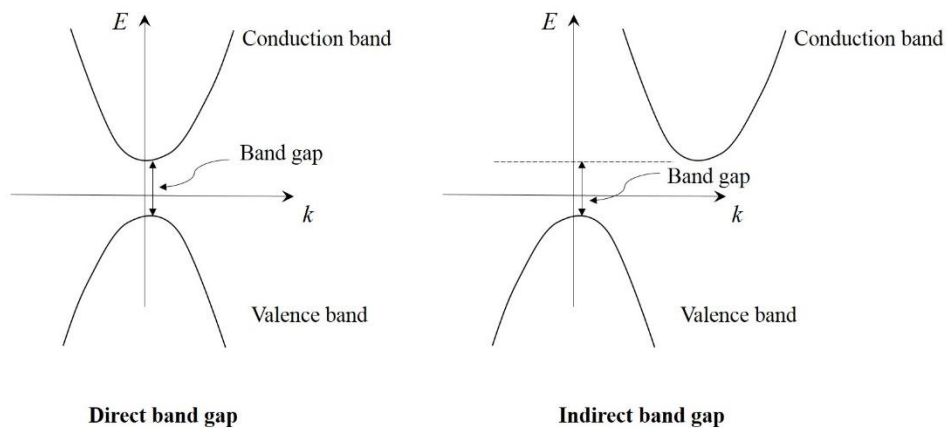
Therefore  $\mathbf{k}$  in the Bloch function does not represent electron momentum.

(iii) From de Broglie's equation  $\lambda = h/p$ , so that the photon momentum at 500 nm wavelength is  $1.3 \times 10^{-27}$  kgm/s.

The Brillouin zone boundary is at  $\pi/a$  or  $0.63 \text{ \AA}^{-1}$ . The crystal momentum  $\hbar\mathbf{k}$  is therefore  $6.6 \times 10^{-25}$  kgm/s.

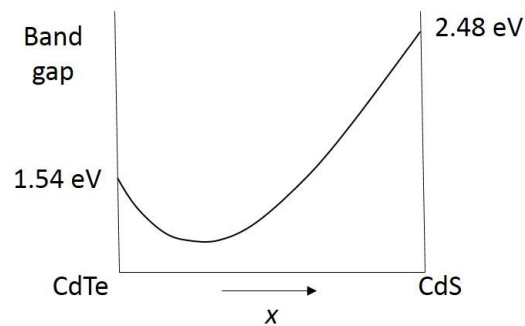
Photon momentum is several orders of magnitude smaller than the crystal momentum. We shall see in the lectures that this has implications for photoabsorption in indirect band gap semiconductors.

(2) (i) Energy-wavevector diagrams:



The photodiode must have a high light absorption coefficient. This is satisfied for direct band gap semiconductors and is therefore the material of choice. Light absorption in indirect band gap semiconductors requires both photon and phonon participation (the latter for momentum conservation) and is therefore weaker.

(ii) The band gap vs. composition curve looks like:



Using  $E = hc/\lambda$  the energy of a 700 nm photon is 1.77 eV. For the solid to be transparent its band gap must be larger than 1.77 eV. We can determine the composition values where the band gap is equal to 1.77 eV, i.e.

$$1.77 = 1.54 - 0.90x + 1.84x^2$$

Solving for  $x$  we get  $x = 0.67$  and  $x = -0.19$ . The latter is not physical (since  $0 \leq x \leq 1$ ) so that from the graph above the composition range is  $0.67 < x \leq 1$ .

(iii) The conduction band minimum and valence band maximum are obtained from  $dE_c/dk = 0$  and  $dE_v/dk = 0$  respectively. The conduction band minimum is at  $k = 1 \text{ m}^{-1}$  and valence band maximum is at  $k = 0 \text{ m}^{-1}$ . The different  $k$ -values mean the band gap is indirect.

Calculating the  $E_c$  and  $E_v$  values at the turning points and taking the difference gives a band gap energy of 1.3 eV.

### Level 3 Condensed Matter Physics- Part II

#### Examples Class 2 Answers

(1) i) Using  $v = (dE/dk)/\hbar$  we get:

$$v = \frac{2Ia}{\hbar} \sin(ka)$$

(ii)  $F = \hbar \frac{dk}{dt} = -e\varepsilon$  gives:

$$k(t) = -\frac{e\varepsilon t}{\hbar}$$

where we have made use of the fact that  $k(0) = 0$ . Substituting in the expression for  $v$ :

$$v(t) = -\frac{2Ia}{\hbar} \sin\left(\frac{ea\varepsilon t}{\hbar}\right)$$

(iii) From  $v = dx/dt$ :

$$x(t) = \frac{2I}{e\varepsilon} \left[ \cos\left(\frac{ea\varepsilon t}{\hbar}\right) - 1 \right]$$

where we have made use of the boundary condition  $x(0) = 0$ . During time averaging the cosine term averages to zero, so that:

$$\langle x \rangle = -\frac{2I}{e\varepsilon}$$

(2) i) Using the fact that  $\mathbf{k}_h = -\mathbf{k}_e$  the  $\mathbf{k}$ -vector for the hole is  $(-0.02, 0, 0) \text{ \AA}^{-1}$ . The energy can be determined by substituting  $\mathbf{k} = (0.02, 0, 0) \text{ \AA}^{-1}$  into the energy expression and noting that the hole energy is the negative of the electron energy. The value is 5.5 meV.

ii) Since  $\nabla_{\mathbf{k}} = (\partial/\partial k_x)\mathbf{i} + (\partial/\partial k_y)\mathbf{j} + (\partial/\partial k_z)\mathbf{k}$  we have to first find the directional derivatives. For a direction  $p$ , where  $p = x, y$  or  $z$ :

$$\frac{\partial E}{\partial k_p} = \frac{\hbar^2}{2m} \left\{ -8.58k_p + \frac{0.92k^2k_p + 23.72k_p(k_q^2 + k_r^2)}{\sqrt{[0.46k^4 + 23.72(k_p^2k_q^2 + k_q^2k_r^2 + k_r^2k_p^2)]}} \right\}$$

where  $k_q$  and  $k_r$  are the  $\mathbf{k}$ -vector components perpendicular to  $k_p$ . For  $\mathbf{k} = (0.02, 0, 0) \text{ \AA}^{-1}$  it is clear that the directional derivative is non-zero only along the  $x$ -direction, so that:

$$\mathbf{v} = -83,543 \text{ \AA} \mathbf{i} \text{ (m/s)}$$

Note that we have used the fact that the hole velocity is equal to the electron velocity.

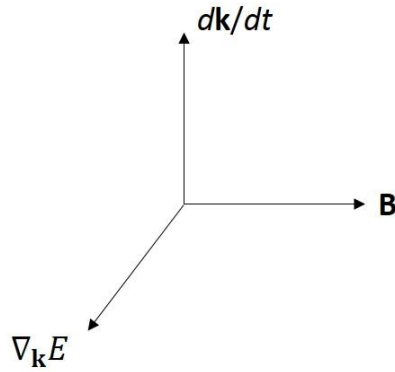
(4) i) introducing the Lorentz force due to the magnetic field:

$$\hbar \frac{d\mathbf{k}}{dt} = q(\mathbf{v} \times \mathbf{B})$$

ii) substituting the expression for the velocity gives:

$$\hbar^2 \frac{d\mathbf{k}}{dt} = q(\nabla_{\mathbf{k}}E \times \mathbf{B})$$

The above equation can be represented diagrammatically as a right-handed system:



Since  $(d\mathbf{k}/dt)$  is perpendicular to  $\mathbf{B}$  this means that the component of  $\mathbf{k}$  parallel to  $\mathbf{B}$  is unchanged. Furthermore the change in energy ( $\delta E$ ) in time  $\delta t$  is given by:

$$\delta E = \frac{dE}{dt} \delta t = \left( \nabla_{\mathbf{k}}E \cdot \frac{d\mathbf{k}}{dt} \right) \delta t = 0$$

Therefore the particle moves along a constant energy surface in  $k$ -space that is perpendicular to  $\mathbf{B}$ .

## Level 3 Condensed Matter Physics- Part II

### Examples Class 3 Answers

(1) (i) Conduction band density of states:

$$g_c(E) = \frac{1}{2\pi^2} \left( \frac{2m_e^*}{\hbar^2} \right)^{3/2} \sqrt{E - E_c}$$

$m_e^*$  is the electron effective mass.

Valence band density of states:

$$g_v(E) = \frac{1}{2\pi^2} \left( \frac{2m_h^*}{\hbar^2} \right)^{3/2} \sqrt{E_v - E}$$

$m_h^*$  is the hole effective mass.

(ii) The Fermi-Dirac distribution function  $f(E)$  is defined as:

$$f(E) = \frac{1}{1 + \exp [(E - \mu)/kT]}$$

The electron concentration ( $n$ ) between energy levels  $E$  and  $E+dE$  is:

$$n(E) = g_c(E)f(E)dE = \frac{1}{2\pi^2} \left( \frac{2m_e^*}{\hbar^2} \right)^{3/2} \frac{\sqrt{E - E_c}}{1 + \exp [(E - \mu)/kT]} dE$$

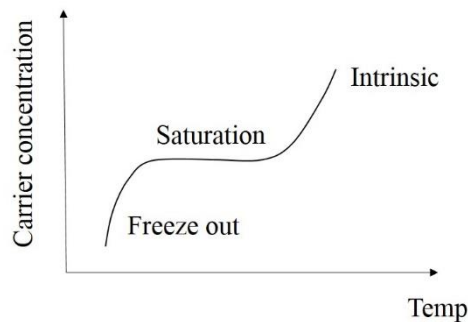
The hole concentration ( $p$ ) between energy levels  $E$  and  $E+dE$  is:

$$p(E) = g_v(E)[1 - f(E)]dE = \frac{1}{2\pi^2} \left( \frac{2m_h^*}{\hbar^2} \right)^{3/2} \frac{\sqrt{E_v - E}}{1 + \exp [(\mu - E)/kT]} dE$$

(iii) Shifting the Fermi level towards the valence band maximum would increase  $(E - \mu)$  for energy levels within the conduction band. Therefore, from the above expression for  $n(E)$  the electron concentration decreases.

On the other hand  $(\mu - E)$  decreases for valence band energy levels and from the expression for  $p(E)$  the hole concentration increases.

(iv)



(v) The Group III impurity has only 3 valence electrons, so substitution in the Group IV semiconductor crystal lattice will effectively generate a hole in the valence band. The majority carriers are therefore holes.

(vi) A diamond cubic crystal structure has 8 atoms per unit cell. The atomic volume density is therefore  $8/[(0.357 \times 10^{-9})^3]$  or  $5.1 \times 10^{28}$  atoms/m<sup>3</sup>.

In the saturation regime every impurity atom is ionised and the majority carrier concentration is approximately equal to the impurity concentration.

Therefore the doping atomic fraction is  $10^{20}/(5.1 \times 10^{28})$  or  $2 \times 10^{-9}$  (2 parts per billion).

(vii) At the intrinsic regime onset the intrinsic carrier concentration ( $n_i$ ) equals the impurity concentration ( $N_o = 10^{20}$  atoms/m<sup>3</sup>). Therefore:

$$n_i = \sqrt{N_c N_v} \exp\left(-\frac{E_g}{2kT}\right) = N_o$$

or  $T = E_g/[k \ln(N_c N_v / N_o^2)]$ . Substituting values gives  $T = \underline{530 \text{ K}}$

(viii) At the onset of freeze out the thermal energy  $kT$  is of the order of the impurity energy level (10 meV). Setting  $kT = 10$  meV gives  $T = \underline{116 \text{ K}}$

Note: a thermal energy of  $(3/2)kT$  is also acceptable, in which case  $T = \underline{77 \text{ K}}$ .

(2) i) Using Gauss' law  $d\varepsilon/dx = \rho(x)/\epsilon_r \epsilon_0$ , where  $\varepsilon$  is the electric field,  $\rho$  the charge density,  $\epsilon_r$  the relative permittivity (static dielectric constant), we have for the  $n$ -side:

$$\varepsilon(x) = \int \frac{\rho(x)}{\epsilon_r \epsilon_0} dx = \int \frac{e N_D x}{\epsilon_r \epsilon_0 w_n} dx = \frac{e N_D}{2 \epsilon_r \epsilon_0 w_n} (x^2 - w_n^2)$$

where the boundary condition that the electric field is zero at the space charge edge  $x = w_n$  has been invoked.

Similarly for the  $p$ -side:

$$\varepsilon(x) = \int \frac{\rho(x)}{\epsilon_r \epsilon_0} dx = - \int \frac{-e N_A x}{\epsilon_r \epsilon_0 w_p} dx = \frac{e N_A}{2 \epsilon_r \epsilon_0 w_p} (x^2 - w_p^2)$$

The extra negative sign in front of the second integral takes into account the fact that ionised acceptors are negatively charged.

Furthermore the electric field within the quasi-neutral regions (i.e.  $x > w_n$  and  $x < -w_p$ ) is zero.

ii) From the continuity of the electric field at  $x = 0$ :

$$e N_D w_n = e N_A w_p$$

This implies charge conservation, since from the dopant profile the condition for equal amounts of positive and negative charge is:

$$\frac{1}{2}eN_Dw_n = \frac{1}{2}eN_Aw_p$$

iii) The potential  $\phi$  is related to the electric field via  $\varepsilon = -(d\phi/dx)$ .

For the  $p$ -side:

$$\phi(x) = - \int \varepsilon(x)dx = \frac{eN_A}{2\epsilon_r\epsilon_0w_p} \int (w_p^2 - x^2)dx = \frac{eN_A}{2\epsilon_r\epsilon_0w_p} \left[ w_p^2x - \frac{(x^3 - 2w_p^3)}{3} \right]$$

where we have arbitrarily set the potential to zero at  $x = -w_p$ .

For the  $n$ -side:

$$\phi(x) = - \int \varepsilon(x)dx = \frac{eN_D}{2\epsilon_r\epsilon_0w_n} \int (w_n^2 - x^2)dx = \phi_{bi} + \frac{eN_D}{2\epsilon_r\epsilon_0w_n} \left[ w_n^2x - \frac{(x^3 + 2w_n^3)}{3} \right]$$

where  $\phi_{bi}$  is the built-in potential at  $x = w_n$ .  $\phi_{bi}$  is equal to the separation of  $n$ - and  $p$ -side Fermi levels within the quasi neutral regions before contact and therefore has the same form as that given in the lectures:

$$\phi_{bi} = \frac{kT}{e} \ln \left( \frac{N_A N_D}{n_i^2} \right)$$

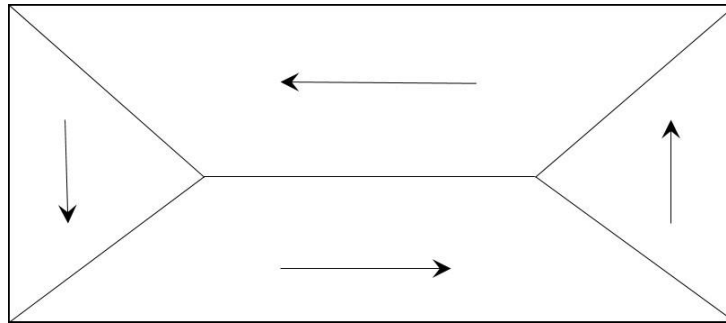
The potential is zero and  $\phi_{bi}$  within the quasi-neutral regions on the  $p$ - and  $n$ -sides respectively.

### Level 3 Condensed Matter Physics- Part II

#### Examples Class 4 Answers

(1) Applying  $B = \mu_0 M_r$ , with  $M_r = 1.72 \times 10^6 \text{ Am}^{-1}$  gives  $B = 2.16 \text{ T}$ . This is considerably larger than the critical magnetic field and therefore a superconducting transition is not expected.

Heating above the Curie temperature and cooling in a zero field will remove the *overall* magnetisation, although within individual magnetic domains (see below) the B-field will be large. Therefore the superconducting transition still cannot take place.

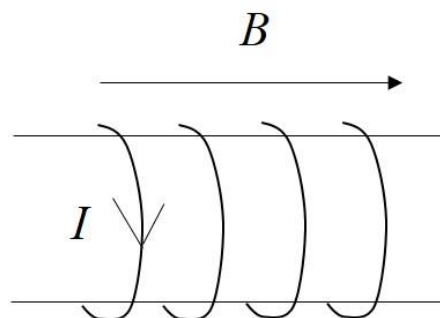


(2) i) For a Type I superconductor:

$$B_c(T) = B_c(0) \left[ 1 - \left( \frac{T}{T_c} \right)^2 \right]$$

Substituting  $B_c(T) = \frac{1}{2} B_c(0)$  gives  $T = T_c/\sqrt{2}$ , the superconducting transition temperature.

ii) The solenoid magnetic field is given by  $B = (\mu_0 NI)/L$ , and is directed along the solenoid axis (see below).



iii) Reversing the direction of the solenoid current will reverse its magnetic field. Therefore we need to select the current direction such that the magnetic field from the solenoid is anti-parallel to the applied field  $\frac{1}{2}B_c(0)$ . At 0 K the maximum B-field that can be generated by the solenoid is therefore  $3B_c(0)/2$ . The maximum current is given by:

$$I_{max} = \frac{3LB_c(0)}{2\mu_0 N}$$



(3) i) Re-arranging for the superconducting electron density gives:

$$n_s = \frac{m}{\mu_o e^2 \lambda_L^2}$$

Substituting values gives  $n_s = 1.4 \times 10^{28}$  electrons/m<sup>3</sup>.

ii) The number of Cooper pairs is  $(n_s/2)$ . If the Cooper pair separation is  $x$  then  $(n_s/2) = 1/x^3$  (imagine a cube of side  $x$  with a Cooper pair at each cube corner. Each Cooper pair contributes  $1/8^{\text{th}}$  to the cube, so there is effectively only one Cooper pair within the cube volume). Using the value for  $n_s$  we obtain  $x = 0.53$  nm as the Cooper pair separation.

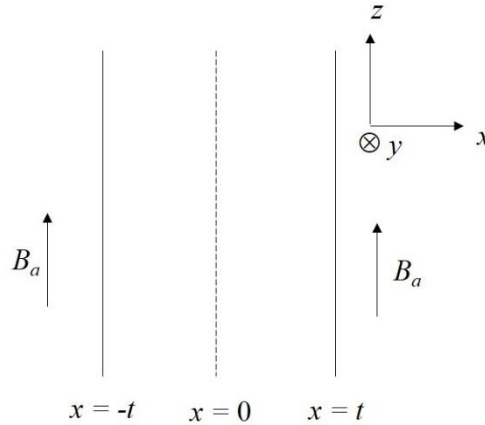
The coherence length for Al is 1550 nm which is much larger than the average Cooper pair separation. It is therefore clear that many Cooper pairs occupy the same region of material.

iii) There are 4 Al atoms within a face centred cubic crystal and therefore 12 valence electrons per unit cell. If  $n_v$  is the density of valence electrons then:

$$n_v = 12/(4.05 \times 10^{-10})^3 = 1.8 \times 10^{29} \text{ electrons/m}^3$$

iv)  $n_v$  is an order of magnitude larger than  $n_s$ . The valence electrons are responsible for atomic bonding, so that only a small fraction can form Cooper pairs while still preserving the structural integrity of the solid.

(4) The slab geometry is indicated below:



Since  $\mathbf{B} = (0,0,B_a)$  the London equation becomes:

$$\frac{d^2 B_z}{dx^2} = \frac{B_z}{\lambda_L^2}$$

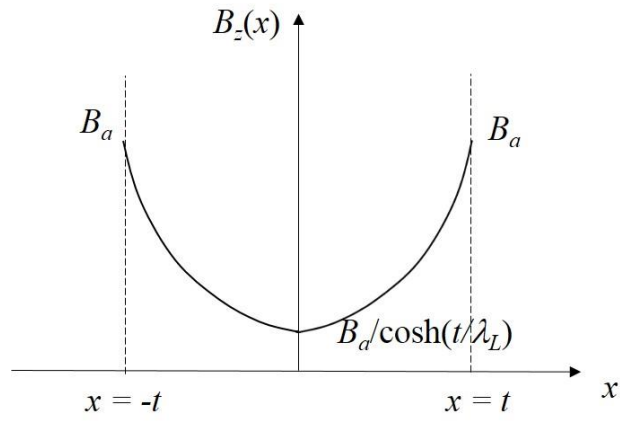
Solutions to this equation are of the form  $B_z(x) = A \exp(x/\lambda_L) + B \exp(-x/\lambda_L)$ , where  $A$  and  $B$  are constants to be determined. From the boundary conditions  $B_z(-t) = B_a$  and  $B_z(t) = B_a$  we find:

$$A = B = \frac{B_a}{\left[ \exp\left(\frac{t}{\lambda_L}\right) + \exp\left(-\frac{t}{\lambda_L}\right) \right]}$$

Using the relation  $\cosh\theta = (e^\theta + e^{-\theta})/2$ , we finally obtain:

$$B_z(x) = B_a \frac{\cosh\left(\frac{x}{\lambda_L}\right)}{\cosh\left(\frac{t}{\lambda_L}\right)}$$

A schematic of the graph is shown below:



### Level 3 Condensed Matter Physics- Part II

#### Examples Class 5 Answers

(1) i) We have:

$$B_c(T) = B_c(0) \left[ \frac{T_c^2 - T^2}{T_c^2} \right]$$

Since  $T$  is close to  $T_c$  we can write  $(T_c^2 - T^2) = (T_c - T)(T_c + T) \approx 2T_c(T_c - T)$ . Substituting this expression gives the desired result.

ii) The condensation energy according to GL theory is  $[\dot{a}(T - T_c)]^2/2b$ . From thermodynamics the condensation energy is  $B_c(T)^2/2\mu_0$ . Equating the two expressions and solving for  $B_c(T)$  we get:

$$B_c(T) = \pm \sqrt{\frac{\mu_0}{b}} \dot{a}(T - T_c)$$

Since  $\dot{a}$  and  $\sqrt{(\mu_0/b)}$  are both positive only the negative solution for  $B_c(T)$  is physically meaningful. We then have:

$$B_c(T) = -\sqrt{\frac{\mu_0}{b}} \dot{a}(T_c - T)$$

This has the same form as the expression in (i).

iii) From the definition of the coherence length:

$$\xi = \left( \frac{\hbar^2}{2m|a(T)|} \right)^{1/2} = \left( \frac{\hbar^2}{2m\dot{a}(T_c - T)} \right)^{1/2}$$

For the London penetration depth we use the fact that the density of superconducting electrons is  $n_s = 2|\psi|^2 = 2\dot{a}(T_c - T)/b$ . Therefore:

$$\lambda_L = \left( \frac{m}{\mu_0 n_s e^2} \right)^{1/2} = \left[ \frac{mb}{2\mu_0 \dot{a} e^2 (T_c - T)} \right]^{1/2}$$

Taking ratios:

$$\kappa = \frac{\lambda_L}{\xi} = \left( \frac{m^2 b}{\mu_0 \hbar^2 e^2} \right)^{1/2}$$

$\kappa$  is therefore independent of temperature and depends only on the GL parameter  $b$ .

iv) For a Type I superconductor  $\kappa < 1$  and for Type II  $\kappa > 1$  (strictly speaking the full GL theory actually predicts  $\kappa < 1/\sqrt{2}$  for Type I and  $\kappa > 1/\sqrt{2}$  for Type II). Therefore:

$$b < \frac{\mu_o \hbar^2 e^2}{m^2} \text{ (Type I)}$$

$$b > \frac{\mu_o \hbar^2 e^2}{m^2} \text{ (Type II)}$$

(2) i) The local magnetisation is  $\mathbf{M}(r) = [\mathbf{B}(r) - \mathbf{B}_a]/\mu_o$ . The magnetic work done per unit volume at the position  $r$  is therefore:

$$W(r) = \int_0^{B_a} \frac{B_a}{\mu_o} \left[ \alpha \left( \frac{R^2 - r^2}{\lambda_L^2} \right) \right] dB_a = \frac{\alpha B_a^2}{2\mu_o \lambda_L^2} (R^2 - r^2)$$

Since  $G_s(r, B_a) = G_s(0) + W(r)$  we obtain the desired result.

ii) Consider a cylinder of unit length. The average magnetic work done per unit volume  $\langle W \rangle$  is defined by:

$$\pi R^2 \langle W \rangle = \int_0^R 2\pi r W(r) dr$$

Substituting the expression for  $W(r)$  and integrating we obtain:

$$\langle W \rangle = \frac{\alpha B_a^2 R^2}{4\mu_o \lambda_L^2}$$

We can therefore express the average free energy per unit volume of the superconductor phase in a magnetic field  $\langle G_s \rangle$  as:

$$\langle G_s \rangle = G_s(0) + \frac{\alpha B_a^2 R^2}{4\mu_o \lambda_L^2}$$

At the critical field  $B_a = B_c$  we have  $\langle G_s \rangle = G_N$ , which leads to the desired result.

iii) At the critical magnetic field the work done by the magnetic field equals the free energy difference between the superconductor and normal states under zero field conditions (a constant).

For a cylinder the average work done by the magnetic field is given by  $\langle W \rangle$ . Compare this to a bulk superconductor, where the magnetic work done is  $B_a^2/2\mu_o$ . We have:

$$\langle W \rangle = \frac{\alpha R^2}{2\lambda_L^2} \left( \frac{B_a^2}{2\mu_o} \right)$$

Since  $R \ll \lambda_L$  it is clear that the critical field for a cylinder will be larger than the bulk superconductor if  $\alpha < 1$ .

(3) i) Using the fact that the magnetic flux passing through the superconducting ring is preserved :

At  $\phi = 0^\circ$  the entire flux  $\Phi$  is provided by the external field. Therefore the supercurrent drops to zero.

At  $\phi = 60^\circ$  the flux through the ring due to the external field is  $\Phi \cos(60^\circ)$  or  $\Phi/2$ . Therefore the remaining  $\Phi/2$  of flux must be provided by a reduced supercurrent of  $(j/2)$ ; note that from the Biot-Savart law the axial magnetic field due to a current carrying loop is proportional to the current.

At  $\phi = 90^\circ$  there is no flux from the external field passing through the ring and the supercurrent is therefore  $j$ .

ii) If the external field is increased to  $3B_a/2$ :

At  $\phi = 0^\circ$  a supercurrent  $j/2$  will flow in the *opposite* sense to cancel the additional flux  $\Phi/2$  from the external field.

At  $\phi = 60^\circ$  the flux through the ring due to the external field is  $(3\Phi/2)\cos(60^\circ)$  or  $3\Phi/4$ . The supercurrent will therefore be  $j/4$ ; the direction of flow is unchanged.

At  $\phi = 90^\circ$  the supercurrent is unchanged since there is no flux from the external field passing through the ring.

### Level 3 Condensed Matter Physics- Part II

#### Supplementary Example Class 5 Answers

(1) Writing  $\mathbf{i}$ ,  $\mathbf{j}$  and  $\mathbf{k}$  for the unit vectors along the  $x$ ,  $y$  and  $z$ -axes, we have  $\boldsymbol{\mu} = \mu\mathbf{j}$ . Furthermore,  $\mathbf{r} = (na)\mathbf{i}$ , where  $\mathbf{r}$  is the position vector between a given dipole at  $x$ -position  $na$  and the origin  $O$  (here  $n$  is any non-zero integer). Since  $\boldsymbol{\mu} \cdot \mathbf{r} = 0$ , the electric field due to a single dipole is:

$$\mathbf{E}(\mathbf{r}) = \frac{-\boldsymbol{\mu}}{4\pi\epsilon_0 r^3}$$

Any electric field at the origin should therefore be parallel to the dipole moment  $\boldsymbol{\mu}$ , i.e. along the  $y$ -axis. Its magnitude is given by:

$$E = -\frac{2\mu}{4\pi\epsilon_0 a^3} \sum_{n=1}^{\infty} \frac{1}{n^3}$$

The additional factor of 2 takes into account dipoles on the left and right hand sides. Substituting the value for  $\Sigma(1/n^3)$  gives  $E = -0.6\mu/(\pi\epsilon_0 a^3)$ . The electric field direction is along the negative  $y$ -axis.

(2) i) The force ( $\mathbf{F}_d$ ) due to damping is  $\mathbf{F}_d = -\gamma m\mathbf{v} = -\gamma m(d\mathbf{r}/dt)$ . Note that since  $\gamma > 0$  a minus sign is used to indicate that the damping acts against the electron velocity  $\mathbf{v}$ . The equation of motion for the electron is therefore:

$$m \frac{d^2 \mathbf{r}}{dt^2} = -K\mathbf{r} - \gamma m \frac{d\mathbf{r}}{dt} - e\mathbf{E}_o \exp(i\omega t)$$

Substituting  $\mathbf{r} = \mathbf{r}_o \exp(i\omega t)$  and solving for  $\mathbf{r}_o$ :

$$\mathbf{r}_o = -\left(\frac{e\mathbf{E}_o}{m}\right) \frac{(\omega_o^2 - \omega^2) - i\gamma\omega}{(\omega_o^2 - \omega^2)^2 + (\gamma\omega)^2}$$

where the substitution  $K = m\omega_o^2$  has been made.

ii) Using the fact that  $\boldsymbol{\mu} = \alpha(\omega)\mathbf{E}_{\text{local}} = -e\mathbf{r}$  gives:

$$-e\mathbf{r}_o = \alpha(\omega)\mathbf{E}_o$$

Substituting the above expression for  $\mathbf{r}_o$  results in:

$$\alpha(\omega) = \left(\frac{e^2}{m}\right) \left[ \frac{(\omega_o^2 - \omega^2)}{(\omega_o^2 - \omega^2)^2 + (\gamma\omega)^2} - i \frac{\gamma\omega}{(\omega_o^2 - \omega^2)^2 + (\gamma\omega)^2} \right]$$

iii) In an undamped medium, where there is no imaginary term in the polarisability, the polarisation ( $\boldsymbol{\mu} = \alpha(\omega)\mathbf{E}_{\text{local}}$ ) of an individual dipole is in phase with the local electric field. In

a damped medium the presence of an imaginary term means that the polarisation is out of phase with the electric field, i.e. the electrons cannot oscillate with the same frequency as the electric field. Effectively this gives rise to an energy loss. Examples of this phenomenon are microwave heating of food and absorption of light by matter.

(3) i) From  $G_{\text{FE}}(T_c) = G_{\text{PE}}(T_c)$  we have:

$$\frac{1}{2}g_2P_c^2 - \frac{1}{4}|g_4|P_c^4 + \frac{1}{6}g_6P_c^6 = \frac{1}{2}P_c^2 \left[ g_2 - \frac{1}{2}|g_4|P_c^2 + \frac{1}{3}g_6P_c^4 \right] = 0$$

Since  $P_c \neq 0$  (ferroelectric phase) the terms within the square brackets must be zero, i.e.

$$g_2 - \frac{1}{2}|g_4|P_c^2 + \frac{1}{3}g_6P_c^4 = 0 \quad \dots (1)$$

ii) From  $d[G_{\text{FE}}(T_c)]/dP = 0$  we have:

$$g_2P_c - |g_4|P_c^3 + g_6P_c^5 = P_c[g_2 - |g_4|P_c^2 + g_6P_c^4] = 0$$

Again since  $P_c \neq 0$  the terms within the square brackets must be zero, i.e.

$$g_2 - |g_4|P_c^2 + g_6P_c^4 = 0 \quad \dots (2)$$

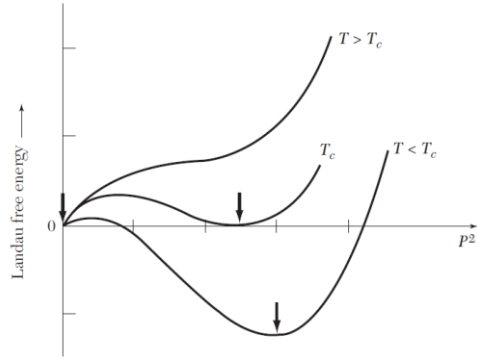
iii) Subtracting (1) from (2) and re-arranging for  $P_c$  gives:

$$P_c = \left( \frac{3|g_4|}{4g_6} \right)^{1/2}$$

iv) The spontaneous polarisation ( $P_s$ ) has the same form as equation (2) with  $P_s$  substituted for  $P_c$ . The roots of the quadratic equation are given by:

$$P_s^2 = \frac{|g_4| \pm \sqrt{|g_4|^2 - 4g_6g_2}}{2g_6}$$

As can be seen from the free energy diagram below the larger value of  $P_s^2$  corresponds to a minimum (the smaller value is a maximum). The spontaneous polarisation is therefore:



$$P_s^2 = \frac{|g_4| + \sqrt{|g_4|^2 - 4g_6g_2}}{2g_6}$$

Or after substituting  $g_2 = \gamma(T - T_o)$ :

$$P_s^2 = \frac{|g_4| + \sqrt{|g_4|^2 - 4g_6\gamma(T - T_o)}}{2g_6}$$

v) At  $T = T_o$  the above equation predicts:

$$P_s(T = T_o) = \left(\frac{|g_4|}{g_6}\right)^{1/2}$$

This is larger than the value of  $P_c$ . Since the spontaneous polarisation of the ferroelectric phase decreases monotonically with temperature (see figure above) this means that  $T_o < T_c$ .