Level 3 Condensed Matter Physics- Part II

Examples Class 1

(1) *Crystal and photon momenta*

(i) Using Bloch's theorem state the form of the electron wavefunction in a periodic crystal potential.

(ii) Using the quantum mechanical operator for momentum show that the Bloch wavevector **k** does not represent the electron momentum (it is in fact the crystal momentum, i.e. electron + lattice)

(iii) Calculate the momentum of a 500 nm wavelength photon.
Calculate the crystal momentum $\hbar\mathbf{k}$ corresponding to the first Brillouin zone of a linear chain of atoms with atom spacing a = 5 Å.
Comment on the magnitude of photon vs crystal momenta.

(2) *Band gap in semiconductors*

(i) Draw separate energy (E)- wavenumber (k) diagrams for a direct and indirect band gap semiconductor. Clearly label the conduction, valence bands and band gap in each diagram.

(ii) The band gap (E_g) in eV of a CdS_xTe_{1-x} alloy is given by:

$$E_g(x) = 1.54 - 0.90x + 1.84x^2$$

Determine the composition range over which the alloy is transparent to light of 700 nm wavelength.

(iii) The energy-wavenumber dispersion relations for the conduction band minimum (E_c) and valence band maximum (E_v) for a particular semiconductor are:

$$E_c(k) = k^2 - 2.0k + 4.3$$

$$E_v(k) = -3.0k^2 + 2.0$$

Where the wavenumber k is in units of m^{-1} and the resulting energy is expressed in units of eV. Calculate the magnitude of the semiconductor band gap and deduce if it is a direct or indirect band gap.

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Examples Class 2
Electrons and Holes

(1) *Conduction of electrons in a perfect crystal*

Consider the band structure of a one-dimensional perfect crystal which has the following dispersion (i.e. E vs k) relation:

$$E(k) = E_0 - 2I\cos(ka)$$

where E_0, I are constants and a is the inter-atomic spacing.

(i) derive an expression for the velocity (υ) of an electron as a function of k.
(ii) using $\mathbf{F} = \hbar(d\mathbf{k}/dt)$ express υ as a function of t when an electric field ε is applied in the positive k-direction (the electric field is applied at $t = 0$; you may assume $k = 0$ at $t = 0$).
(iii) show that the time averaged position of the electron is given by $\langle x \rangle = -(2I/e\varepsilon)$, where e is the charge of the electron (assume that $x = 0$ at $t = 0$)

The result in part (iii) reinforces the fact that electrons in a perfect crystal cannot carry a current (i.e. scattering is required for electrical conduction).

(2) *Properties of holes*

The valence band in silicon has the following dispersion relation:

$$E(\mathbf{k}) = \frac{\hbar^2}{2m}\left\{-4.29k^2 + \sqrt{\left[0.46k^4 + 23.72(k_x^2k_y^2 + k_y^2k_z^2 + k_z^2k_x^2)\right]}\right\}$$

where m is the rest mass of the electron.

Assume a photon promotes an electron at $\mathbf{k} = (0.02, 0, 0)$ Å^{-1} into the conduction band, leaving behind a hole.

For the hole calculate:

(i) the corresponding **k**-vector and energy
(ii) its velocity (use the vector form of the group velocity, $\mathbf{v} = (1/\hbar)\nabla_{\mathbf{k}}E$, where $\nabla_{\mathbf{k}}$ is the ∇ operator evaluated in reciprocal space)

(3) *Charge carriers in a magnetic field*

(i) Using $\mathbf{F} = \hbar(d\mathbf{k}/dt)$ write down an equation for the motion of particle of charge q and velocity $\mathbf{v}$ in a magnetic field $\mathbf{B}$.
(ii) By making use of the fact that $\mathbf{v} = (1/\hbar)\nabla_{\mathbf{k}}E$ show that the particle moves along a constant energy surface in k-space that is perpendicular to $\mathbf{B}$.

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Examples Class 3
Topic: Semiconductor doping and pn-junctions

(1) *Semiconductor doping*

The density of states $g(E)$ at energy E for a free electron metal is given by:

$$g(E) = \frac{1}{2\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\sqrt{E}$$

where m is the electron mass.

Consider a semiconductor in equilibrium with chemical potential μ, minimum conduction band energy E_c and maximum valence band energy E_v.

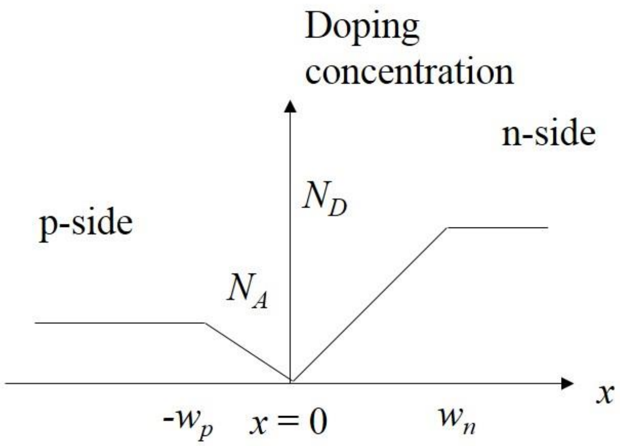
(i) Using the free electron metal density of states write down equivalent expressions for the conduction and valence band density of states in the semiconductor.
(ii) Derive expressions for the equilibrium electron and hole concentrations between energies E and $E+dE$, where dE is a small energy increment.
(iii) If the chemical potential is shifted towards the valence band how would the electron and hole concentrations change?

A Group III impurity is now added to the Group IV intrinsic semiconductor.

(iv) Sketch the variation in majority carrier concentration as a function of temperature clearly labelling the different regimes.
(v) In the saturation regime are the majority carriers electons or holes?
(vi) Calculate the percentage concentration of impurity atoms that must be added in order to achieve a majority carrier concentration of 10^{20} carriers/m^3 in the saturation regime. Assume the semiconductor has a diamond cubic crystal structure with 5.4 Å lattice parameter.
(vii) Calculate the temperature at which the semiconductor shows intrinsic behaviour. Assume $E_g = 1.1$ eV, $N_c = 2.8 \times 10^{25}$ m^{-3} and $N_v = 1.0 \times 10^{25}$ m^{-3}, where N_c is the effective density of states for the conduction band and N_v is the effective density of states for the valence band.
(viii) If the impurity energy level within the band gap is 10 meV estimate the temperature below which impurity freeze-out takes place.

(2) *pn-junctions*

Consider a pn-junction with the following doping profile, where the donor, acceptor concentrations increase linearly from zero within the space charge region and are constant within the quasi-neutral regions:



The donor, acceptor concentrations at the space charge edges on the *n*-side ($x = w_n$) and *p*-side ($x = -w_p$) are N_D and N_A respectively. Assuming equilibrium and the depletion approximation:

(i) Calculate the electric field distribution within the device.
(ii) By comparing the electric field at $x = 0$ show that charge is conserved for this device.
(iii) Calculate the electrostatic potential as a function of position x.

Level 3 Condensed Matter Physics- Part II

Examples Class 4
Topic: Superconductors in magnetic fields

(1) *Superconductivity and ferromagnetism*

Iron has a saturation magnetisation (M_s) of 1.72 x 10^6 Am^{-1}. In Type I elemental superconductors the critical magnetic field is typically found to be smaller than 0.1 T.

Using Fe as an example discuss the possibility of ferromagnetic materials becoming superconducting at low temperatures (you may assume that the remnance magnetisation has a similar value to M_s).

Assume now that Fe is heated above the Curie temperature and cooled in a zero magnetic field, so that it has zero magnetisation. Would the material become superconducting at low temperature?

(2) *Critical currents and fields*

A Type I superconductor is cooled from room temperature under a magnetic field ½$B_c(0)$, where $B_c(0)$ is the critical magnetic field at 0 K.

i) At which temperature will the normal to superconducting transition be observed? You may express the result in terms of the zero field transition temperature T_c.
ii) Write down an expression for the magnetic field generated by a solenoid with (N/L) number of turns per unit length and carrying a current I. You may refer to old lecture notes or the web.
iii) If the solenoid is made of the superconducting material in part (i) calculate the maximum current that can be carried at 0 K without destroying the superconducting state, assuming the external magnetic field ½$B_c(0)$ is applied along the solenoid axis.
[*Hint*: pay attention to the current direction- does this have an effect on the critical current?]

(3) *London Penetration depth*

The formula for the London penetration depth λ_L is given by:

$$\lambda_L = \sqrt{\frac{m}{\mu_0 n_s e^2}}$$

where μ_0 is the permeability of free space, m,e the mass and charge of an electron and n_s is the number density of superconducting electrons.

Aluminium is a Type I superconductor with T_c value of 1.2 K. λ_L for Al at 0 K temperature is measured to be 45 nm.

i) Calculate the density of superconducting electrons at 0K.
ii) Calculate the average spacing between Cooper pairs.
iii) Al has a face centred cubic crystal structure with lattice parameter 4.05 Å. Calculate the density of valence electrons (There are 3 valence electrons per Al atom).
iv) Compare the result of (iii) with (i). Why is it important that the density of valence electrons is larger than superconducting electrons?

(4) *London equation- slab of finite thickness*

The London equation describes the penetration of a magnetic field **B** into a superconductor and is given by:

$$\nabla^2 \mathbf{B} = \frac{\mathbf{B}}{\lambda_L^2}$$

where λ_L is the London penetration depth (a constant). Consider a superconducting slab of thickness $2t$. The plane of the slab is in the yz-plane and an external field B_a is applied in the z-direction. Show that the magnetic field within the slab is given by:

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

where $x = 0$ passes through the centre of the slab. Sketch the shape of this function.

Level 3 Condensed Matter Physics- Part II

Examples Class 5
Topic: Thermodynamics of Superconductors

(1) *Ginzburg-Landau model*

In the Ginzburg-Landau (GL) model the Gibbs free energy for a homogeneous superconductor (G_s) in a magnetic field free environment is expressed as:

$$G_s(T) = G_N(T) + a(T)|\psi|^2 + \frac{b}{2}|\psi|^4$$

where G_N is the free energy of the normal phase and $a(T) = \dot{a}(T - T_c)$, with $\dot{a} > 0$. Due to the limited number of terms in the Taylor expansion the GL model is only valid close to T_c.

i) The critical magnetic field for a Type I superconductor is given by:

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

Show that close to T_c the critical magnetic field is approximately:

$$B_c(T) \approx \frac{2B_c(0)}{T_c}(T_c - T)$$

ii) Starting from the expression for condensation energy derive an expression for $B_c(T)$ using GL-theory. Show that this is consistent with the approximation in (i).

iii) Express the superconductor coherence length (ξ) and London penetration depth (λ_L) in terms of the constants $\dot{a}$ and b in the GL model (please refer to notes for definitions of ξ and λ_L). From this show that GL theory predicts the ratio $\kappa = \lambda_L/\xi$ to be temperature independent.

iv) Using your result for κ express the conditions for Type I and Type II behaviour in terms of the GL model parameters $\dot{a}$ and b.

(2) *Magnetic energy in superconductors*

A superconducting cylinder with radius $R << \lambda_L$ is placed in an external magnetic field $\mathbf{B}_a$. The magnetic field within the cylinder can be approximated by:

$$\mathbf{B}(r) = \mathbf{B}_a\left(1 + \alpha\frac{r^2}{\lambda_L^2} - \alpha\frac{R^2}{\lambda_L^2}\right)$$

where α is a constant.

i) Using the expression for magnetic work done per unit volume $dW = -\mathbf{M} \cdot d\mathbf{B}_a$ and the relation $\mathbf{B}(r) = \mathbf{B}_a + \mu_o \mathbf{M}$, show that the Gibbs free energy density of the superconducting phase in the cylinder is given by:

$$G_s(r, B_a) = G_s(0) + \frac{\alpha B_a^2}{2\mu_o \lambda_L^2}(R^2 - r^2)$$

where $G_s(0)$ is the free energy density at zero applied field.

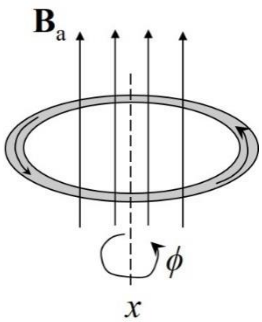
ii) At the critical field B_c the average free energy across the cylinder $\langle G_s \rangle$ is equal to the free energy of the normal state G_N. Show that this leads to the condition:

$$G_N - G_s(0) = \frac{\alpha B_c^2 R^2}{4\mu_o \lambda_L^2}$$

iii) If $\alpha<1$ is the critical magnetic field for the cylinder smaller or larger than the bulk superconductor?

(3) *Flux through a superconductor ring*

A superconducting ring in the *xy*-plane has a persistent current (magnitude *j*) which generates a magnetic field $\mathbf{B}_a$ along the z-direction. A feature of superconductivity is that the magnetic flux passing through the ring must be constant (magnetic flux is the **B**-field integrated over the area enclosed by the ring). The ring can be rotated about the *x*-axis through an arbitrary angle ϕ. After rotation an external magnetic field is applied along the z-direction with the same magnitude as $\mathbf{B}_a$.



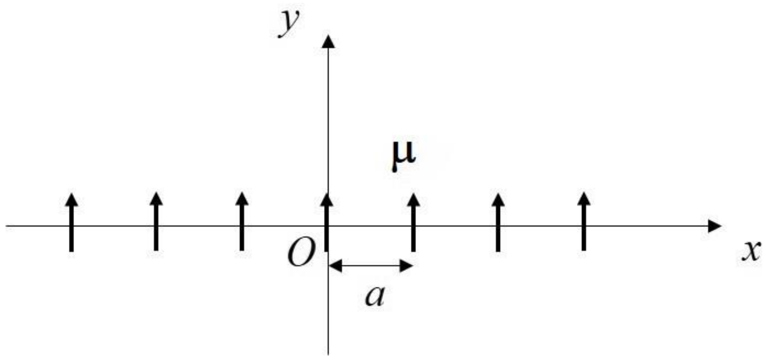
(i) Using the fact that the magnetic flux is constant determine the supercurrent for $\phi = 0^o$ (starting position), 60^o and 90^o. Express your answer in terms of the supercurrent *j* before the external field was applied.

(ii) What would the supercurrents for the different ϕ-values be if the external field was still along the z-direction but had a larger magnitude of $(3B_a/2)$?

Level 3 Condensed Matter Physics- Part II
Supplementary Examples Class (Topic: Dielectrics)

(1) *Electric dipole moments*

Consider an infinite one dimensional row of electric dipoles as shown below. The moment for each dipole is $\boldsymbol{\mu}$ and is in the direction of the positive y-axis. The dipoles are arranged regularly along the x-axis with spacing 'a'. Calculate the electric field experienced by the dipole at the origin O due to all other dipoles.



[*Hint*: (i) the electric field due to a single dipole is $(\mathbf{r}) = \frac{3(\boldsymbol{\mu}\cdot\mathbf{r})\mathbf{r}-r^2\boldsymbol{\mu}}{4\pi\epsilon_o r^5}$, (ii) $\sum_{n=1}^{\infty}\frac{1}{n^3} \approx 1.2$

(2) *Electronic polarisation in a damped medium*

Assume polarisation of the electron cloud of an atom under a local electric field $\mathbf{E}_o\exp(i\omega t)$ can be modelled as simple harmonic motion (SHM) of a spring with spring constant $K = m\omega_o^2$. Assume also that the system is damped (this can happen through, say, electron-electron collisions). In SHM the damping force is proportional to the linear momentum of the oscillating particle. Hence we can define a positive constant $\gamma = F_d/mv$, where F_d and v are the magnitudes for the damping force and velocity respectively, while m is the particle mass.

i) Write down the equation of motion for the position $\mathbf{r}$ of the oscillating electron taking into account damping. By substituting $\mathbf{r} = \mathbf{r}_o\exp(i\omega t)$ solve this equation for $\mathbf{r}_o$.

ii) Show that the polarisability $\alpha(\omega)$ is given by:

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

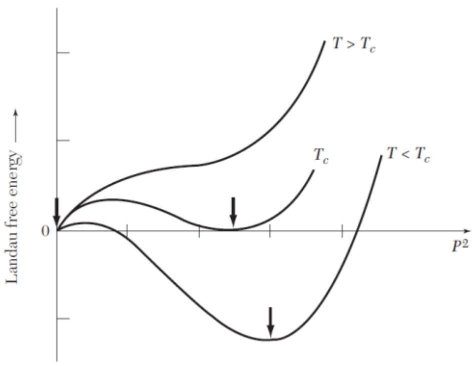
iii) The polarisability has an imaginary term compared to an undamped system. Comment on the physical significance of this extra term.

(3) *Ginzburg-Landau theory of first order ferroelectric transitions*

The Ginzburg-Landau free energy for a first order transition in the absence of an electric field is given by:

$$G_{FE}(T) = G_{PE}(T) + \frac{1}{2}g_2P^2 - \frac{1}{4}|g_4|P^4 + \frac{1}{6}g_6P^6$$

where $g_2 = \gamma(T\text{-}T_o)$ and γ, T_o, $g_6 > 0$. The free energy curves as the temperature passes through the Curie transition temperature are shown schematically below:



At the Curie temperature T_c the free energy of the ferroelectric phase is equal to the paraelectric phase.

i) By setting $G_{\mathrm{FE}}(T_c) = G_{\mathrm{PE}}(T_c)$ write down a polynomial equation for the ferroelectric polarisation P_{c} at the Curie temperature.

ii) By setting $d[G_{\mathrm{FE}}(T_c)]/dP = 0$ write down another polynomial equation for P_{c}.

iii) Using the two previous expressions show that:

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

iv) Show that the spontaneous polarisation P_{s} in the ferroelectric state at temperature T is given by:

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

v) By comparing P_{s} at $T = T_o$ with the expression for P_c show that $T_o < T_c$ for a first order transition.