

2012

PAPER 7 (Quantum Condensed Matter Physics) – ANSWERS

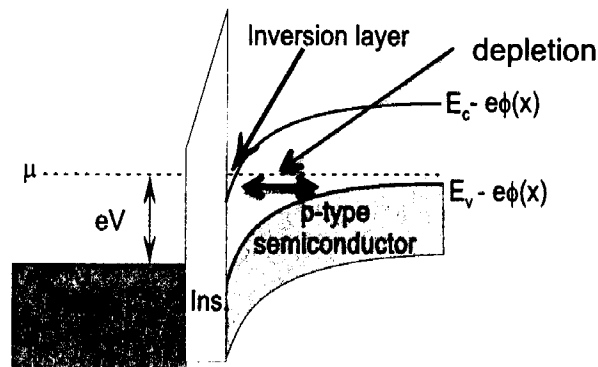
1 Attempt **all** parts of this question. Answers should be concise, and relevant formulae may be assumed without proof.

(a) sketch the valence and conduction energy levels in a metal/insulator/p type semiconductor structure under conditions where an n-type inversion layer just forms, indicating also the depletion regime.

[4]

Solution:

The diagram below is extracted from the lecture overheads, with the addition of the identification of the depletion regime.



(b) The wave function of the electron associated with a donor atom in a semiconductor can be treated as a modified hydrogenic state. For a semiconductor with effective mass, $m^* = 0.1m_e$ and relative dielectric constant of 12, calculate the effective Bohr radius and the density of dopants at which the orbitals overlap.

[4]

Solution:

The Bohr radius, a_0 is given by

$$a_0 = \frac{4\pi\epsilon\epsilon_0\hbar^2}{me^2}$$

[2 marks for stating or deriving this result]

substituting values, $a_0 = 5.4 \times 10^{-2}$ nm for the H atom, and 6.5 nm for the semiconductor electron wave function.

to calculate the density, $n \text{ m}^{-3}$ of donor wave functions of radius 6.5 nm at which overlap occurs take a cubic lattice (approximate but ok here), so

$$n = \left(\frac{1}{2 \times 6.5 \times 10^{-19}} \right)^3 = 4.6 \times 10^{23} \text{ m}^{-3}$$

(18 April 2012)

(c) A one-dimensional material has an energy band $E(k)$ described by a one-dimensional tight-binding model

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

where the lattice constant $a = 0.3$ nm. Calculate the value of the transfer integral, t , required to make the effective mass at the bottom of the band equal to the electron mass. [4]

Solution: We can expand the energy near $k = 0$ as

$$E(k) = E_0 - 2t + tk^2a^2$$

We set tk^2a^2 equal to $\hbar^2k^2/2m_e$ to give $t = \hbar^2/2a^2m_e$ ($=\hbar^2/2a^2m_e e$ in eV) = 0.4 eV.

2 *Attempt this question. Credit will be given for well-structured and clear explanations, including appropriate diagrams and formulae. Detailed mathematical derivations are not required.*

Write brief notes on **two** of the following: [13]

(a) photovoltaic solar cells and the Shockley-Queisser efficiency limit

Solution:

- photovoltaic solar cells comprise a semiconductor with a band gap selected to absorb the visible and some of the IR solar spectrum
- absorbed photons produce electron hole pairs that can be collected at appropriate electrodes with chemical potentials that match those of electrons and holes, often provided by p-doped and n-doped regions (with silicon). Flow of electron and hole currents driven by diffusion and drift (when away from open circuit).
- Shockley-Queisser limit - maximum energy conversion efficiency for a single junction solar cell, around 33%. Trade-off between fraction of solar spectrum absorbed (lower band gap) against maximum open-circuit voltage (limited by semiconductor band gap). Optimum band gap around 1.5 eV
- credit will be given for extra material, including the mention of practical semiconductors (silicon, GaAs, CIGS, CdTe), or mention of higher efficiencies using tandem cells.

(b) methods for measuring band structure

Solution:

- photoemission. UV photon absorbed produces a photo emitted electron. Its kinetic energy determines its binding energy with respect to the vacuum level, and the energy dependence of photoemission intensity gives a measure of the valence band density of states.
- the angular dependence of photoemission can also provide information about the k dependence of the photo emitted electron. This allows two-dimensional slices of the energy band dispersion to be measured
- optical absorption provides some information (though it depends on the density of states of both valence and conduction bands).
- Fermi surfaces can be mapped out using magnetic field quantisation of energy levels, measured through oscillations in susceptibility, resistance etc.
- electron tunnelling across narrow barriers, as with scanning tunnelling microscopes, depends on density of available states for tunnelling.

(c) magnetic properties of materials

Solution:

- credit for mention of Part 1B coverage of diamagnetism
- paramagnetism associated with electron spins. isolated spins give Curie law temperature dependence ($1/T$)
- electrons in metals - Pauli principle reduces paramagnetic response by $k_B T/E_F$ to give temperature-independent susceptibility.
- exchange interaction, U causes spin ordering - which can be ferro- or antiferro-magnetic
- ferromagnetic metals - Stoner criterion for transition from para- to ferro-magnetism, $N(E)U > 1$.

3 Attempt **either** this question **or** question 4.

For a nearly free electron gas subject to a periodic potential of the form $V(\mathbf{r}) = 2V_G \cos(\mathbf{G} \cdot \mathbf{r})$ the electronic energy levels $E(\mathbf{k})$ for wavevectors \mathbf{k} close to the relevant Brillouin zone boundary ($\mathbf{kG} \simeq |\mathbf{G}|^2/2$) are described by

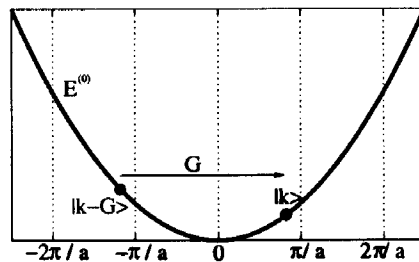
$$E(\mathbf{k}) = \frac{\hbar^2 \mathbf{k}^2 + (\mathbf{k} - \mathbf{G})^2}{2m} \pm \left(\left(\frac{\hbar^2 \mathbf{k}^2 - (\mathbf{k} - \mathbf{G})^2}{2m} \right)^2 + |V_G|^2 \right)^{1/2}$$

• Outline the derivation of this result.

[5]

Solution: Bookwork - relevant lecture overhead is set out below. A reasonable answer would include a sketch showing the coupling of k states separated by \mathbf{G} , an indication of the trial wave functions and the use of perturbation theory.

- **Example: 1D case.** Start with state $|\mathbf{k}\rangle$. Potential V_G admixes $|\mathbf{k} - \mathbf{G}\rangle$, which is close in energy. It also admixes other states, but their energies are more widely separated from that of $|\mathbf{k}\rangle$, so we concentrate on $|\mathbf{k} - \mathbf{G}\rangle$ for now.



- **Apply H to $|\psi\rangle$:**

$$|\psi\rangle = \alpha_{\mathbf{k}} |\mathbf{k}\rangle + \alpha_{\mathbf{k}-\mathbf{G}} |\mathbf{k} - \mathbf{G}\rangle$$

$$\mathbf{H} |\psi\rangle = E |\psi\rangle = \alpha_{\mathbf{k}} \frac{p^2}{2m} |\mathbf{k}\rangle + \alpha_{\mathbf{k}} V |\mathbf{k}\rangle + \alpha_{\mathbf{k}-\mathbf{G}} \frac{p^2}{2m} |\mathbf{k} - \mathbf{G}\rangle + \alpha_{\mathbf{k}-\mathbf{G}} V |\mathbf{k} - \mathbf{G}\rangle$$

- **Left multiply with basis states $\langle \mathbf{k} |$ and $\langle \mathbf{k} - \mathbf{G} |$:**

$$\alpha_{\mathbf{k}} E = \alpha_{\mathbf{k}} E_{\mathbf{k}}^{(0)} + \alpha_{\mathbf{k}-\mathbf{G}} V_G$$

$$\alpha_{\mathbf{k}-\mathbf{G}} E = \alpha_{\mathbf{k}} V_{-\mathbf{G}} + \alpha_{\mathbf{k}-\mathbf{G}} V_0 + \alpha_{\mathbf{k}-\mathbf{G}} E_{\mathbf{k}-\mathbf{G}}^{(0)}$$

(Note $E_{\mathbf{k}}^{(0)} = \hbar^2 k^2 / 2m$, V_0 is set to zero, and $V_{-\mathbf{G}} = V_{\mathbf{G}}^*$).

- **Obtain 2 perturbed energies E from roots of 2×2 determinant.**
 Extended zone scheme: call one energy $E_{\mathbf{k}}$ and the other $E_{\mathbf{k}-\mathbf{G}}$.
 Reduced zone scheme: call one energy $E_{\mathbf{k}}^{(1)}$ and the other $E_{\mathbf{k}}^{(2)}$.
- **At Brillouin zone boundary ($k = \pi/a$), $E = E_{\pi/a}^{(0)} \pm |V_G|$**

- Discuss how this result can explain the existence of energy bands separated by energy gaps in crystalline lattices

[3]

Solution:

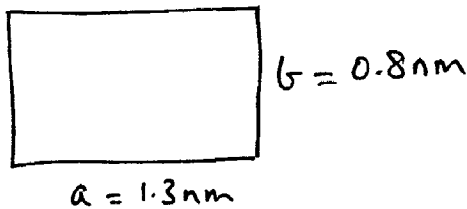
Energy gaps of modulus $2|V_G|$ are opened at the Brillouin zone boundary. If the gaps opened at all points on the Brillouin zone boundary are sufficiently large, then an energy gap can be opened so that all states in the lower band are at lower energies than all states in the upper band.

- In a certain material, electronic motion along one of the crystalline axes is strongly suppressed, giving rise to a free electron gas with a two-dimensional dispersion

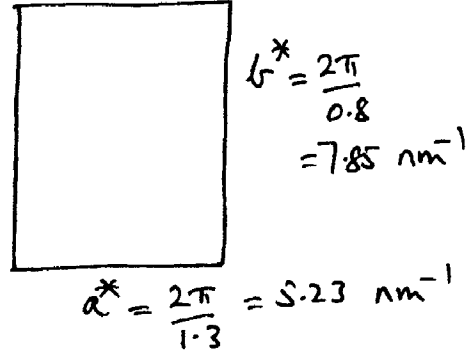
$$E^{(0)}(\mathbf{k}) = \frac{\hbar^2}{2m} (k_x^2 + k_y^2)$$

The unit cell is rectangular, with dimensions $a = 1.3 \text{ nm}$ and $b = 0.8 \text{ nm}$. Draw a labelled sketch of the real space and the reciprocal space unit cell, indicating for the latter the first Brillouin zone.

[3]

Solution:

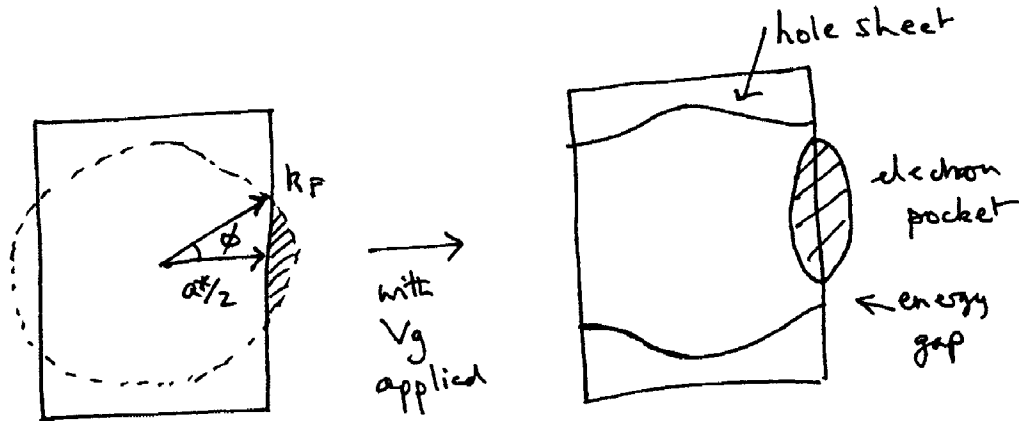
real space



reciprocal space

• There are two mobile electrons per rectangular unit cell. Remembering that the first Brillouin zone contains a sufficient number of states to accommodate two electrons per unit cell, sketch the Fermi surface for the free-electron gas, showing that it extends beyond the first Brillouin zone. Show how in the presence of the lattice potential the circular Fermi surface is split into two open sheets and one closed sheet. [4]

Solution:



• Deduce an upper limit on the cross-sectional area of the closed sheet. [3]

Solution:

The areas of the Brillouin zone and Fermi circle are equal, so $\pi k_F^2 = b^* c^*$ giving $k_F = 3.62 \text{ nm}^{-1}$.

From the diagram above $\cos \phi = a^*/2k_F = .722$ making ϕ close to $\pi/4$. Electron pocket area is twice the shaded area in left-hand figure above, this is equal to

$$2k_F^2(\phi - \sin \phi \cos \phi)$$

With ϕ equal to $\pi/4$, the area of the pocket is 7.5 nm^{-2}

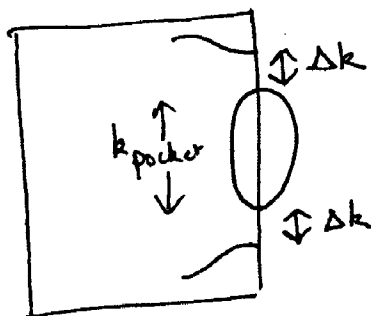
• Resistivity measurements in high magnetic fields reveal quantum oscillations. The frequency of these oscillations corresponds to a cross-sectional area $A_k = 5.74 \text{ nm}^{-2}$. Show that this result is consistent with your estimate of the cross-sectional area of the closed sheet. [4]

Solution:

Magnetic field oscillations give an area that is smaller than the 'free electron' area, so the electron pocket has shrunk due to the opening of a gap at the Brillouin zone boundary. This is illustrated in the right-hand sketch above.

- Assuming that the chemical potential is the same as when $V_G = 0$, make a rough estimate in eV of $|V_G|$. [3]

Solution:



In the sketch above, we note that the energies of carriers on the electron and hole Fermi surfaces separated by Δk must be equal. There are several ways to approach this calculation - and a very crude approach is to set the free electron energy difference across this gap to $2V_G$. This gives

$$\frac{\hbar^2}{2m_e} ((k_F + \Delta k/2)^2 - (k_F - \Delta k/2)^2) = \frac{\hbar^2}{m_e} k_F \Delta k = 2V_G$$

How to estimate Δk ? if the contraction in the pocket area scales as k_{pocket}^2 then Δk is about 12.5% of k_F , giving a value for V_G of about 80 meV.

4 Attempt **either** this question **or** question 3.

- Describe the use of the Lorentz oscillator model to describe the optical response due to electrons in semiconductors and insulators. [4]

Solution: Bookwork. The use of the Lorentz oscillator model to describe electronic response in semiconductors and insulators gives a semiclassical description of the electronic transitions, from valence to conduction band states, treating these as forced simple harmonic oscillators. It is possible to add contributions from many oscillators at different frequencies to model the range of electronic transition energies observed in real semiconductors..

- Show that the frequency dependence of the dielectric response, $\epsilon(\omega)$ is given by

$$\epsilon(\omega) = 1 + \frac{ne^2}{\epsilon_0 m} \frac{1}{\omega_0^2 - \omega^2 - i\omega\gamma}$$

where n is the number density of participating electrons of charge e and mass m , ω_0 is the resonant frequency of the oscillator and γ is the damping rate. [4]

Solution: Bookwork. Solutions will be based on the lectured material set out below:

- Electron cloud behaves as damped harmonic oscillator

$$m\ddot{u} + m\gamma\dot{u} + m\omega_T^2 u = qE$$

(ω_T = natural frequency, given by force constant and mass; γ = damping rate).

- Consider oscillating electric field $E(t) = E_\omega e^{-i\omega t}$, which induces oscillating displacement $u(t) = u_\omega e^{-i\omega t}$.
- Resulting dipole moment per atom at angular frequency ω : $p_\omega = qu_\omega$
- Polarisation = dipole moment density: $P_\omega = \epsilon_0 \chi_\omega E_\omega$, with

$$\chi_\omega = \frac{N}{V} \frac{q^2}{m\epsilon_0(\omega_T^2 - \omega^2 - i\omega\gamma)}$$

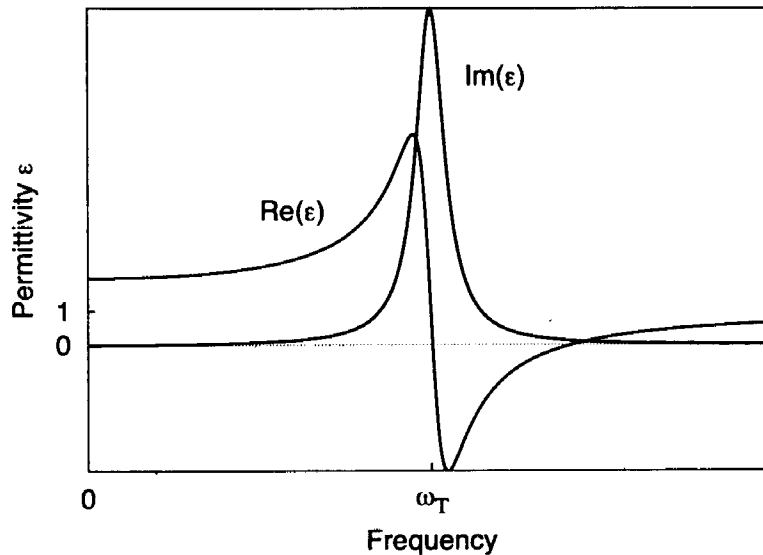
- Permittivity $\epsilon_\omega = 1 + \chi_\omega$.

• Sketch $\Re[\epsilon(\omega)]$ and $\Im[\epsilon(\omega)]$ as a function of ω for a finite value of ω_0 and discuss how these account for optical reflection and absorption.

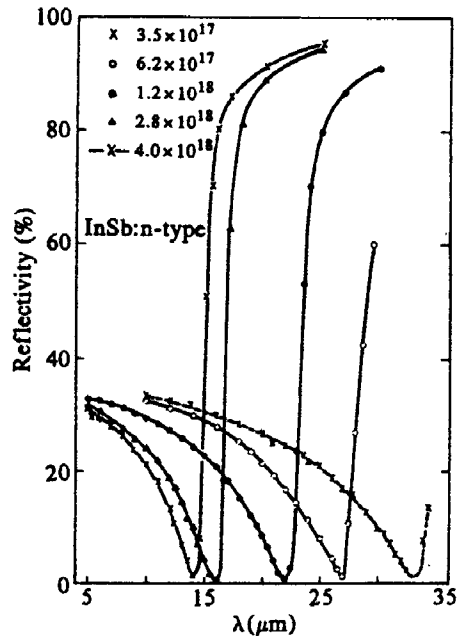
[4]

[You may wish to use the result that the (power) reflectivity $R = \left| \frac{\sqrt{\epsilon}-1}{\sqrt{\epsilon}+1} \right|^2$.]

Solution: Bookwork. Solutions will be based on the scheme shown in lectures set out below:



- at low frequencies - little absorption, but significant reflection because the low frequency dielectric constant is raised above 1 by the sub-resonant response of the oscillator.
- near resonance - significant absorption associated with the imaginary part of the dielectric constant associated with the damping term, γ .
- at high frequencies - little reflection and absorption.



The graph shows R versus wavelength λ for an extrinsically doped semiconductor, InSb, which has a semiconductor band gap of around 0.2 eV , with different free carrier concentrations as indicated (in units of cm^{-3}).

- Noting that at short wavelengths R reaches a value of 35%, estimate the value of the low frequency dielectric constant [2]

Solution: R at $5\mu\text{m} = 35\%$ (note that a wavelength of $5\mu\text{m}$ is about 0.25 eV , close to the band gap). Substitution into

$$R = \left| \frac{\sqrt{\epsilon} - 1}{\sqrt{\epsilon} + 1} \right|^2$$

gives $\epsilon = 15$.

- The lattice parameter for the conventional cubic unit cell of InSb, which contains 4 units of InSb, is 0.56nm . If four electrons per InSb contributes to the Lorentz oscillator used to describe the optical response of the valence electrons, calculate the value of the plasma frequency, in eV that these electrons would show if free, $\omega_p^2 = ne^2/\epsilon_0 m$. [3]

Solution:

Plasma frequency for valence electrons in InSb:
number density of carriers, n with 4 electrons per unit cell
 $n = \frac{16}{(5.6 \times 10^{-8})^3}$ gives $\omega_p^2 = 5 \text{ eV}$.

- What value of ω_0 accounts for the observed low frequency dielectric constant? Comment on this value in relation to the actual band gap. [4]

Solution:

Given that $\epsilon = 15$ at low frequencies, where $\epsilon = 1 + \omega_p^2/\omega_0^2$ we require $\omega_0 = 1.3 \text{ eV}$. This value is considerably higher than the minimum band gap for InSb, but is representative of the average energy of optical transitions involving the valence electrons.

- By considering the optical response at longer wavelengths to be the sum of the free carrier response of the carriers introduced by doping and valence electrons, described as above, explain why the reflectivity reaches a minimum before rising to a high value at long wavelengths. [4]

Solution:

Adding free electrons with effective mass m^* provided by extrinsic doping, with density n_e gives a further, free-electron contribution to $\epsilon(\omega)$ of $-n_e e^2 / \epsilon_0 m^*$.

The reflectivity minimum occurs when $\epsilon(\omega) = 1$ and the rise in reflection at longer wavelengths is due to the free carrier reflectivity of the extrinsic charges below their plasma frequency.