Chapter 10 Problems

10.1 Preliminaries

1. Prove Bloch's theorem. This was done in lectures in PH22006 (Bloch states) by considering a plane wave in one dimension as a starting point.

2. Prove $E(k)$ is periodic in reciprocal lattice vectors g for the electron states of a crystalline material. This was also done in lectures in PH22006.

3. From Fig. 2.5 and Fig. 2.4, confirm that GaP is a semiconductor, discuss its electron and hole effective masses near $k = 0$ (the diagram's not quite good enough to measure them), find its speeds of sound, and find the lowest photon energy at which GaP starts to absorb or emit light. You will need the lattice parameter of GaP, which is 5.4505 Å.

4. Check the phonon frequencies of Fig. 2.6 agree with those in Fig. 2.5 and identify which is the LO mode and which is the TO mode.

5. Prove Eq. (2.7). Not examinable but very worthwhile!

6. Considering a potential with just two Fourier components (i.e, considering two plane waves k and $k - G$), use degenerate perturbation theory to prove that $E_g = 2V_G$. [A lot of work].

7. Consider two hydrogen atoms (1 and 2) with s orbitals $|1\rangle$ and $|2\rangle$. Find the energies of the molecular bonding and antibonding orbitals Ψ given the following assumptions. You should obtain $E = E_0 \pm \beta$. (should be easy).

- Write Ψ as $\Psi = c_1|1\rangle + c_2|2\rangle$ (which is not normalised)
- Require $\langle 1|2\rangle = \langle 2|1\rangle = 0$ (not generally true)
- $\langle 1|H|1\rangle = \langle 2|H|2\rangle = E_0$
- $\langle 1|H|2\rangle = \langle 2|H|1\rangle = \beta$

8. Following the previous question, now allow 'hopping' between atoms by setting

- $\langle 1|2\rangle = \langle 2|1\rangle = S$ where $S \to 0$ as $r \to \infty$.

and find the new energies (hard). You will need to use the variational principle ($\partial E/\partial c_{1,2} = 0$) to obtain simulataneous equations for $c_{1,2}$ and solve a determinant equation for their coefficients. You should find that:

$$E = \frac{E_0 \pm \beta}{1 \pm S}.$$

9. For the *fcc* lattice, the lattice point at $(0,0,0)$ has 12 neighbours at positions:

$$r = \frac{a}{2}(\pm 1, \pm 1, 0), \frac{a}{2}(\pm 1, 0 \pm 1), \frac{a}{2}(0, \pm 1, \pm 1)$$

In the nearest-neighbour tight-binding model, show that an equation for the energy band is

$$E(k) = E_0 - \beta - 4\gamma \left(\cos(k_x a/2)\cos(k_y a/2) + \cos(k_y a/2)\cos(k_z a/2) + \cos(k_z a/2)\cos(k_x a/\right.$$

Plot this energy band along the path $L - \Gamma - X - K - \Gamma - W$ in reciprocal space, where

$$\begin{aligned} L &= (1/2, 1/2, 1/2) \\ \Gamma &= (0,0,0) \\ X &= (1,0,0) \\ K &= (3/4, 3/4, 0) \\ W &= (1, 1/2, 0) \end{aligned}$$

A Jupyter notebook is probably a good tool for doing this.

10. Show that the form of EQ.(3.16) is correct. A starting point is to recognise that, in 1D, the density of states in k is a constant.

10.2 Optical coefficients

1. Show (without using section 2.1) that the energy of a photon with wavelength λ, measured in microns, is E, measured in electron volts, such that $E = 1.24\lambda$.
2. The reflectivity of silicon at 633 nm is 35% and the absorption coefficient is $3.8 \times 10^5 \text{m}^{-1}$. Calculate the transmission of a sample with a thickness of 10 μm at this wavelength (see Fig.5.2). [$T = 0.0095$]

3. Crown glass has a refractive index of 1.51 in the visible spectral region. Calculate the reflectivity of the air-glass interface (always assume normal incidence unless otherwise indicated), and the transmission through a typical glass window. [$R = 0.041, T = 0.92$]

4. A material has a reflectivity of 0.15 and an absorption coefficient α of 100 cm^{-1}. Design a shield that will permit only 1% of the incident radiation to be transmitted through the material.

5. The semiconductor gallium arsenide (GaAs) has a refractive index of 3.68 and an absorption coefficient of 1.3×10^6 m^{-1} at 800 nm. Calculate the transmission coefficient of a 2.0 μm thick GaAs sample at this wavelength. [$T = 0.034$]

6. Sea water has a refractive index of 1.33 and absorbs 99.8% of red light of wavelength 700 nm in a depth of 10 m. What is its complex dielectric constant at this wavelength? [$\tilde{\varepsilon}_r = 1.77 + 9.2 \times 10^{-8} i$]

7. Estimate the reflectivity of a silver mirror at a wavelength of 100 μm. You may assume that $\varepsilon_2 >> |\varepsilon_1|$. The conductivity of silver is $6.6 \times 10^7 \Omega^{-1}$m. [99.6%]

8. Explain why an induced polarization of the form $P(t) = \alpha E(t) + \beta E^2(t)$ can lead to the production of frequency doubled light if the re-radiated field is proportional to d^2P/dt^2. [not discussed in lectures & not examinable!]

9. The complex dielectric constant of the semiconductor CdTe is given by $\varepsilon_r = 8.92 + 2.29i$ at 500 nm. Calculate the phase velocity of light, the absorption coefficient and the reflectivity at normal incidence. Is CdTe a weak or strong absorber at this wavelength?

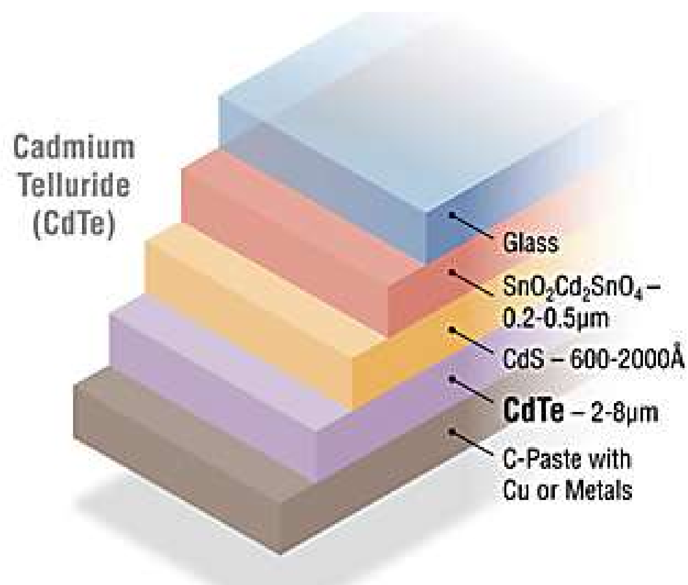

Figure 10.1: Structure of a CdTe-based solar cell: note how thin the active CdTe layer is compared to an equivalent silicon-based solar cell (which is a few hundred microns thick).

10.3 Lorentz oscillator model

1. A beam of light passes through a gas with an atomic density of 10^{17} m^{-3}. The full width at half maximum of an atomic absorption line in the gas at 589 nm is 100 MHz. Calculate the peak absorption coefficient.

2. In the dipole oscillator model the equation of motion is:

$$m_0 \frac{d^2x}{dt^2} + m_0\gamma\frac{dx}{dt} + m_0\omega_0^2 x = -eE(t) \tag{10.1}$$

Sketch the phase relationship between the polarization $P(t)$ and the driving field $E(t)$.

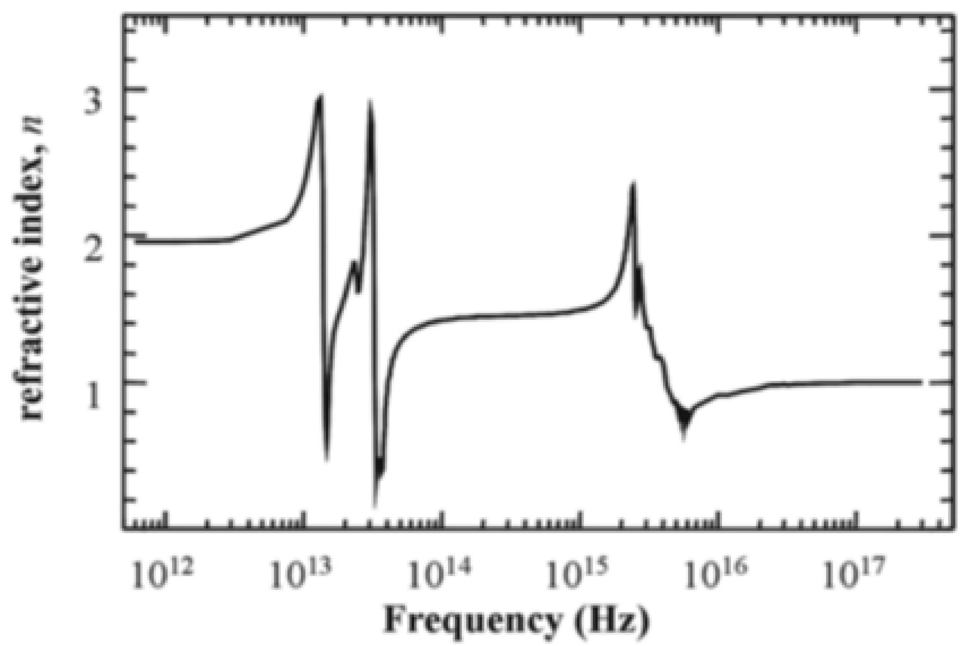

Figure 10.2: Refractive index of fused silica.

$$\tilde{\varepsilon}_r(\omega) = \varepsilon_\infty + (\varepsilon_{st} - \varepsilon_\infty)\frac{\omega_0^2}{(\omega_0^2 - \omega^2 - i\gamma\omega)} \tag{10.2}$$

3. For Eq. (10.2) and Fig. 10.2:

- Define the variables in the equation;
- Account for the shape of the graph;
- Draw a sketch of the extinction coefficient over the same frequency range;
- Estimate the reflectivity of fused silica at a wavelength of 1.0 μm;
- Estimate the extinction coefficient, κ, of fused silica at 3×10^{15} Hz.

4. The dielectric constant of a system with a single undamped atomic resonance is

$$\varepsilon_r(\omega) = 1 + \frac{Ne^2}{\varepsilon_o m_o} \frac{1}{(\omega_o^2 - \omega^2)}. \tag{10.3}$$

   Show that the group velocity is always less than c.

5. Show that for a weakly absorbing resonance (assume $\varepsilon_2 << \varepsilon_1$) the absorption coefficient at the line centre of a Lorentz oscillator does not depend on the value of ω_0.

6. A sapphire crystal doped with titanium absorbs strongly around 500nm. Calculate the difference in the refractive index of the doped crystal above and below the 500nm absorption band if the density of the absorbing atoms is 1×10^{25} m^{-3}. The refractive index of undoped sapphire is 1.77. Note, you can use the Lorentz model with N equal to the dopant number density and the background index equal to that of the sapphire. [6.3×10^{-4}]

7. In the Lorentz oscillator model,

$$\varepsilon_2(\omega) = \frac{Ne^2}{\varepsilon_0 m_0} \frac{\gamma\omega}{(\omega_0^2 - \omega^2)^2 + (\gamma\omega)^2}.$$

   Show that the full width at half maximum of the peak in ε_2 is γ (assume $\gamma << \omega_0$).

8. The greenhouse gas carbon dioxide gives rise to a strong dip in the atmospheric infrared solar transmission spectrum at a wavelength of 4.3 μm due to excitation of vibrations of the CO_2 molecule. If the peak absorption coefficient at sea level is 0.8 m^{-1} and the molecular absorption can be modelled as a Lorentz oscillator estimate the concentration of CO_2 in parts per million. Assume an oscillator strength of 0.5, full width at half maximum of the absorption line of 160 cm^{-1} and that the CO_2 molecule can be treated as a carbon atom bound to a single oxygen atom. The density of air at sea level is 1.2 kgm^{-3} and the mass of C, O and N atoms are 12, 16 and 14 amu respectively. [1700 ppm]

10.4 Plasmas and plasmons

1. Calculate the doping density at which the bulk plasmons in n-type GaAs have the same frequency as the longitudinal optic phonon at 297 cm^{-1} if $m_e^* = 0.067 \times m_0$ and the optical refractive index is 3.3.

2. Ignoring damping, what is the $\omega(k)$ relationship (that is, the photon dispersion curve) for light in a metal?

3. The frequency dependence of the relative dielectric constant of a gas of free electrons is given by

$$\varepsilon_r(\omega) = 1 - \frac{\omega_p^2}{\omega^2 + i\gamma\omega}$$

where ω is the angular frequency, γ is the damping rate, and ω_p is the plasma frequency defined by $\omega_p = \sqrt{(}Ne^2/\epsilon_0 m_e)$. N is the number of electrons per unit volume, e the electron charge, ϵ_0 the permittivity of free space and m_e the free electron mass.

a. Explain why metals are expected to have nearly 100% reflectivity for frequencies below the plasma frequency. (Hint: assume weak damping)
b. Zinc is a divalent metal with 6.6×10^{28} m^{-3} atoms per unit volume. Account for the shiny appearance of zinc. [λ_p=92 nm: reflective in visible]
c. The ionosphere reflects radio waves with frequencies of up to about 3 MHz, but transmits waves with higher frequencies. Estimate the free electron density in the ionosphere. [$N \sim 10^{11}$m^{-3}]

4. Caesium metal is found to be transparent to electromagnetic radiation of wavelengths below 440 nm. Calculate a value for the electron effective mass. For caesium: $N = 0.91 \times 10^{28}$ m^{-3}. [$m^* = 1.6m_e$]

5. The momentum scattering time of silver is 4.0×10^{-14} s at room temperature. Calculate the dielectric constant at 500 nm, neglecting interband absorption effects. Hence, estimate the reflectivity of a silver mirror at this wavelength. The plasma frequency for silver is 2.17×10^{15} Hz. [R=99.6%]

6. Using the Drude-Lorentz model, estimate the fraction of light with wavelength 1.0 μm that is transmitted through a 20 nm thick gold film at 77 K, where the DC electrical conductivity is 2.0×10^8 Ω^{-1}m^{-1}. The plasma frequency and electron density of gold are $N = 5.9 \times 10^{28}$ m^{-3} and $\omega_p = 1.37 \times 10^{16}$ rad/s. [Ignoring surface reflections: T=0.16]

7. What is the value of ε for a medium with zero reflectivity? Use the expression for $\varepsilon(\omega)$ for a doped semiconductor to find an expression for the frequency with zero reflectivity. (Hint: set the damping to zero). Use the data shown in the figure to find the value of the electron effective mass of InSb for the lowest (0.35×10^{24} m^{-3}) and highest (4.0×10^{24} m^{-3}) carrier densities. Take $\varepsilon_{opt} = 15.6$.

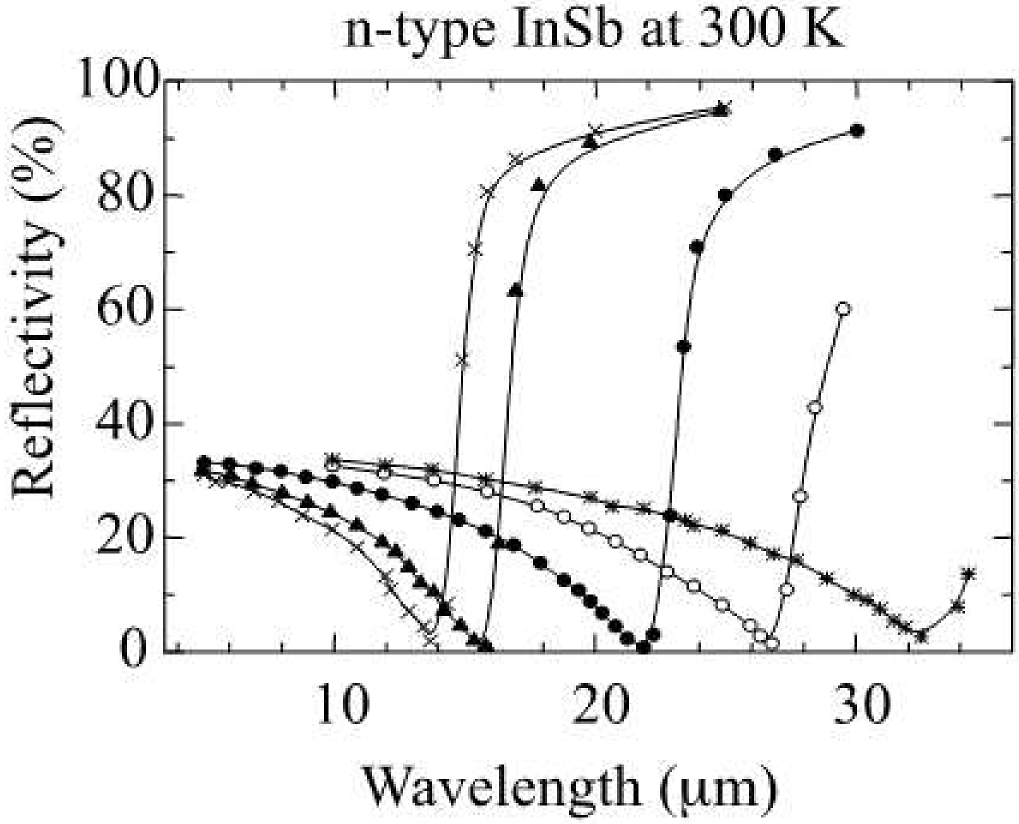

Figure 10.3: After Fox, fig 7.7

8. Plasmons can be modelled as a collective mode of the whole electron gas as one object. The figure below shows a schematic view of a charge cloud (free carrier density N) displaced by distance u, thus generating an electric field $E = Neu/\varepsilon_0$. Write down and solve an equation of motion for this oscillating charge cloud and show that the frequency of oscillation is the plasma frequency ω_p obtained by a different route above (Eq. (8.3).

10.5 Lattice vibrations

1. Estimate the absorption coefficient at the TO phonon frequency in a polar solid with damping constant $\gamma = 10^{11}$ s^{-1} if $\Omega_{TO} = 2\pi \times 10^{13}$ rad/s, $\varepsilon_{st} = 12.1$ and $\varepsilon_\infty = 10.0$

2. The static and high frequency dielectric constants of LiF are $\varepsilon_{st} = 8.9$ and $\varepsilon_\infty = 1.9$ respectively. The TO phonon frequency ν_{TO} is 9.2 THz. Calculate the upper and lower wavelengths of the reststrahlen band. [15-33 μm]

3. Estimate the reflectivity in the middle of the reststrahlen band (you may just assume a frequency of 10.5 THz if you wish) from a crystal with ν_{TO} =10 THz, $\varepsilon_{st} = 12.1$ and $\varepsilon_\infty = 10$, when the damping constant γ is (a) 10^{11} s^{-1} and (b) 10^{12} s^{-1}. [Answer: 98%, 84%. Note that greater damping reduces the reflectivity]

4. In an inelastic light scattering experiment on silicon using an laser at 514.5 nm, Raman peaks are observed at 501.2 nm and 528.6 nm. Account for the origin of the two peaks, and estimate their intensity ratios if the sample temperature is 300 K. [Phonon at 15.5, 0.08]

References

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