Part III Advanced Quantum Condensed Matter Physics

Question sheet III

1. **Joint density of states in 1 and 2 dimensions**
   Calculate the joint density of states between a parabolic valence band maximum, and a parabolic conduction band minimum, both centered at k = 0, in 2 and 1 dimensions (the calculation for 3 dimensions was done in the lectures). Comment on the significance of your results on the shape of the absorption spectrum of semiconductors of different dimensions near the band edge.

$$E_c(k) - E_v(k) = E_g + \frac{\hbar^2 k^2}{2m_e^*} + \frac{\hbar^2 k^2}{2m_h^*} = E_g + \frac{\hbar^2 k^2}{2m^*} \quad \text{with} \quad \frac{1}{m^*} \equiv \frac{1}{m_e^*} + \frac{1}{m_h^*}$$

$$\vec{\nabla}_k \left(E_c(k) - E_v(k)\right) = \frac{\hbar^2 k}{m^*}$$

$$\text{In 3D: } J_{cv}(\omega) = \frac{2}{(2\pi)^3}\left[\frac{4\pi k^2}{\hbar^2 k} m^*\right]_{k=\sqrt{\frac{2m^*}{\hbar^2}(\hbar\omega - E_g)}} = \frac{1}{2\pi^2}\left(\frac{2m^*}{\hbar^2}\right)^{3/2}\sqrt{\hbar\omega - E_g}$$

$$\rho(\varepsilon) = \frac{2}{(2\pi)^d}\int dk \frac{m^* k^{d-1}}{\hbar^2 k} = \begin{cases} \frac{\sqrt{2}\left(m^*\right)^{3/2}}{\pi^2\hbar^3}\sqrt{\varepsilon} & \text{in 3D} \\ \frac{m^*}{\pi\hbar^2} & \text{in 2D} \\ 2\sqrt{\frac{2m}{\varepsilon\hbar^2}} & \text{in 1D} \end{cases}$$

   S: Only 2 discrete points in 1D, circle in 2D

2. **Excitons in semiconductors**
   Write a brief essay on the different descriptions of Mott-Wannier and Frenkel excitons in semiconductors, and discuss examples of systems where the two types of excitons can be observed.

   Mott-Wannier exciton : radius larger than lattice constant, hydrogenic model can be used, example: direct band gap semiconductors with large dielectric constant and/or small effective mass (GaAs)

   Frenkel exciton: radius comparable to lattice constant, molecular description appropriate, semiconductors with small dielectric constant and/or large effective mass (organic semiconductors, ionic crystals)

3. **Refractive index of GaAs**

At 4 K the n = 1 exciton in GaAs has a peak absorption coefficient of $3\cdot 10^6$ m^{-1} at 1.5149 eV with a full width at half maximum equal to 0.6 meV. By applying the Lorentz oscillator model to the exciton, determine the magnitude and energy of the local maximum in the refractive index just below the exciton absorption line. The non-resonant refractive index of GaAs at energies below the band gap is 3.5.

Hint: Use the Lorentz oscillator model in the approximate form, which is valid close to the resonance:

$$\varepsilon_1(\Delta\omega) = \varepsilon_\infty - (\varepsilon_{static} - \varepsilon_\infty)\frac{2\omega_T \Delta\omega}{4(\Delta\omega)^2 + \gamma^2}$$

$$\varepsilon_2(\Delta\omega) = (\varepsilon_{static} - \varepsilon_\infty)\frac{\gamma\omega_T}{4(\Delta\omega)^2 + \gamma^2}$$

$$\Delta\omega = \omega - \omega_T \quad \varepsilon_\infty = \varepsilon(\omega \to \infty) \quad \varepsilon_{static} = \varepsilon(\omega = 0) \quad \gamma = 1/\tau$$

Calculate the frequency at which the maximum in ε_1 occurs, and then use the information on the peak absorption coefficient to calculate ε_∞.

Lorentz oscillator model:

$$\varepsilon_2(\Delta\omega) = (\varepsilon_{st} - \varepsilon_\infty)\frac{\gamma\omega_T}{4(\Delta\omega)^2 + \gamma^2}$$

$$\varepsilon_1(\Delta\omega) = \varepsilon_\infty - (\varepsilon_{st} - \varepsilon_\infty)\frac{2\omega_T\Delta\omega}{4(\Delta\omega)^2 + \gamma^2}$$

ε_1 has a maximum just below $\Delta\omega = 0$. Its position can be obtained from:

$$\frac{d\varepsilon_1}{d\omega} = \frac{d\varepsilon_1(\Delta\omega)}{d\Delta\omega} \propto \frac{16\omega_T\Delta\omega^2 - 2\omega_T\left(4(\Delta\omega)^2 + \gamma^2\right)}{\left(4(\Delta\omega)^2 + \gamma^2\right)^2} = 2\omega_T\,\frac{4\Delta\omega^2 - \gamma^2}{\left(4(\Delta\omega)^2 + \gamma^2\right)^2}$$

Maximum at $\Delta\omega = -\frac{\gamma}{2}$

$$n = \sqrt{\frac{1}{2}\left(\varepsilon_1 + \sqrt{\varepsilon_1^2 + \varepsilon_2^2}\right)}$$

$$\varepsilon_1\left(\Delta\omega = -\frac{\gamma}{2}\right) = \varepsilon_\infty + (\varepsilon_{st} - \varepsilon_\infty)\frac{\omega_T}{2\gamma}$$

$$\varepsilon_2\left(\Delta\omega = -\frac{\gamma}{2}\right) = (\varepsilon_{st} - \varepsilon_\infty)\frac{\omega_T}{2\gamma}$$

$$\varepsilon_{st} = (3.5)^2 = 12.25$$

$$\omega_T = 2.301\cdot 10^{15}\,Hz$$

$$\gamma = 9\cdot 10^{11}\,Hz$$

$$\alpha_{\max} = \frac{4\pi k}{\lambda} \Rightarrow k = 3\cdot 10^6 \cdot 818.5nm/4\pi = 0.195$$

$$k^2 = \frac{1}{2}\left(-\varepsilon_\infty + \sqrt{\varepsilon_\infty^2 + (\varepsilon_0 - \varepsilon_\infty)^2\,\frac{\omega_T^2}{\gamma^2}}\right)$$

$$(2k^2 + \varepsilon_\infty)^2 = 4k^4 + 4k^2\varepsilon_\infty + \varepsilon_\infty^2 = \varepsilon_\infty^2 + \varepsilon_0^2\,\frac{\omega_T^2}{\gamma^2} - 2\varepsilon_0\varepsilon_\infty\,\frac{\omega_T^2}{\gamma^2} + \varepsilon_\infty^2\,\frac{\omega_T^2}{\gamma^2}$$

$$\varepsilon_\infty^2\,\frac{\omega_T^2}{\gamma^2} - 2\varepsilon_0\varepsilon_\infty\,\frac{\omega_T^2}{\gamma^2} - 4k^2\varepsilon_\infty + \varepsilon_0^2\,\frac{\omega_T^2}{\gamma^2} - 4k^4 = 0$$

$$\varepsilon_\infty^2 - \varepsilon_\infty\left(2\varepsilon_0 + 4k^2\,\frac{\gamma^2}{\omega_T^2}\right) + \varepsilon_0^2 - 4k^4\,\frac{\gamma^2}{\omega_T^2} = 0$$

$$\varepsilon_\infty = \left(\varepsilon_0 + 2k^2\,\frac{\gamma^2}{\omega_T^2}\right) \pm \sqrt{\left(\varepsilon_0 + 2k^2\,\frac{\gamma^2}{\omega_T^2}\right)^2 - \varepsilon_0^2 + 4k^4\,\frac{\gamma^2}{\omega_T^2}} = 12.2495$$

$$n_{\max} = \sqrt{\frac{1}{2}\left(\varepsilon_1 + \sqrt{\varepsilon_1^2 + \varepsilon_2^2}\right)} = 3.59$$

Alternative solution:

Make the approximation of weak absorption from the start (k<<n):

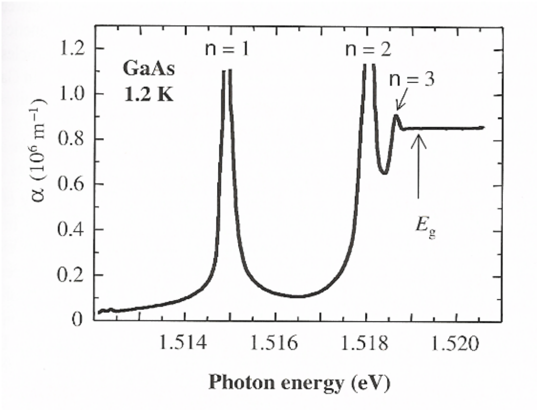
$\varepsilon_1 = n^2 \quad \varepsilon_2 = 2nk$

Using these two relationships facilitates the algebra somewhat.

4. Excitons in GaAs

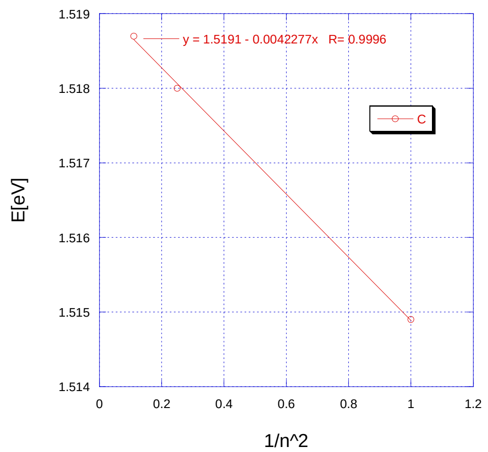
The graph below shows the optical absorption spectrum for GaAs as a function of energy (in eV). Quantum numbers corresponding to the hydrogenic bonding model have been assigned. Use these data to estimate:

- the band gap;
- the average effective mass for electrons and holes [use a value of 10 for the relative permittivity];



Absorption spectrum of GaAs at 1.2 K near the band edge.

Plot Energy vs $1/n^2$:

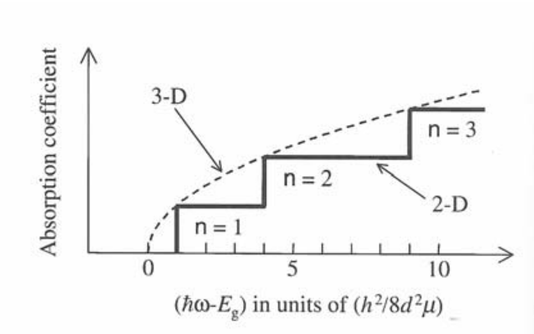


The band gap can be read from the y-axis intercept: 1.5191 eV

$$\text{Slope}: 0.0042 = \frac{13.6eV}{\varepsilon^2}\frac{\mu}{m} \Rightarrow \mu = 0.03 = \left(\frac{1}{m_e} + \frac{1}{m_h}\right)^{-1}$$

5. Optical absorption in quantum wells

(a) The figure below shows a comparison of the joint density of states of a 2D and a 3D semiconductor with parabolic bands. Show that the JDOS of the 2D system is equal to that of the 3D system at the bottom of each of the subbands.



(b) Estimate the difference in the wavelength of the absorption edge of bulk (3D) GaAs and a 20 nm GaAs quantum well (assume infinite well size). What is the difference in the onset of absorption for transitions from the heavy hole and the light-hole band in the quantum well ? (The band gap of bulk GaAs is 1.424eV at room temperature.)

(a) We need to compare JDOS for equivalent volumes in 2D and 3D. In 3D we consider a volume of area A and thickness d.

$$\rho(\varepsilon) = \frac{2}{(2\pi)^d}\int dk \frac{m^* k^{d-1}}{\hbar^2 k} = \begin{cases} Ad\frac{\sqrt{2}\left(m^*\right)^{3/2}}{\pi^2\hbar^3}\sqrt{\varepsilon} & \text{in 3D} \\ A\frac{m^*}{\pi\hbar^2} & \text{in 2D} \end{cases}$$

$$E_n = \frac{\hbar^2}{2m_e^*}\left(\frac{n\pi}{d}\right)^2 + \frac{\hbar^2}{2m_h^*}\left(\frac{n\pi}{d}\right)^2 = \frac{\hbar^2}{2m^*}\left(\frac{n\pi}{d}\right)^2$$

$$\rho_{3D}(E_n) = n\frac{m^*}{\pi\hbar^2}$$

(b)

$m_{hh}^* = 0.53 m_e \quad m_{lh}^* = 0.08 m_e \quad m_e^* = 0.067 m_e$

$$E_{hh1} = \frac{\hbar^2}{2m_{hh}^*}\left(\frac{n\pi}{d}\right)^2 = 2meV$$

$$E_{lh1} = \frac{\hbar^2}{2m_{lh}^*}\left(\frac{n\pi}{d}\right)^2 = 12meV$$

$$E_{e1} = \frac{\hbar^2}{2m_{lh}^*}\left(\frac{n\pi}{d}\right)^2 = 14meV$$

$$E_g + E_{e1} + E_{hh1} = 1.44eV \quad \rightarrow \quad \lambda[nm] = \frac{1240}{E[eV]} = 861nm$$

$$E_g + E_{e1} + E_{lh1} = 1.450eV \quad \rightarrow \quad \lambda[nm] = \frac{1240}{E[eV]} = 855nm$$

$$E_g = 1.424eV \quad \rightarrow \quad \lambda[nm] = \frac{1240}{E[eV]} = 871nm$$

6. **Selection rules for optical absorption in a 2D quantum well**

In a quantum well system one cannot only have transitions between a hole subband and an electron subband, but also transitions in between two hole subbands. (These occur typically in the mid- to far-infrared, and are used for example in infrared lasers, such as quantum cascade lasers.)

Consider the matrix element for an intersubband transition between the n-th and the n'-th subband of a quantum well for light polarized in the z-direction perpendicular to the planes of the quantum well.

$$M_{nn'} = \int_{-\infty}^{\infty} \varphi_n^*(z) z \varphi_{n'}(z) dz$$

(a) Show that for $M_{nn'}$ to be non-zero $\Delta n = n - n'$ must be an odd number.

Z is an odd function, so the matrix element will be zero, unless the wavefunctions for n and n' have different parities, ie., $\Delta n = n - n'$ must be an odd number.

(b) Compare the relative strengths of the 1 → 2 and the 1 → 4 transitions in a 20 nm GaAs electron quantum well with infinite barriers. What is the wavelength of the 1 → 2 transition ($m_e^* = 0.067\ m_e$) ?

$$\varphi_n(z) = \sqrt{\frac{2}{d}} \sin\left(k_n z + \frac{n\pi}{2} \right)$$

$$M_{1\to 2} == \frac{2}{d} \int_{-d/2}^{d/2} \sin\left(\frac{\pi z}{d} + \frac{\pi}{2} \right) z \sin\left(\frac{2\pi z}{d} + \pi \right)$$

$$z' = z + d/2$$

$$M_{1\to 2} = \frac{2}{d} \int_0^d \sin\left(\frac{\pi z'}{d} \right) z' \sin\left(\frac{2\pi z'}{d} \right) = \frac{2}{d} \left. \frac{d\left(9d \cos\left(\frac{\pi z}{d} \right) - d \cos\left(\frac{3\pi z}{d} \right) + 12\pi z \sin\left(\frac{\pi z}{d} \right)^3 \right)}{18\pi^2} \right|_0^d$$

$$= -\frac{16}{9\pi^2} d$$

$$M_{1\to 4} = \frac{2}{d} \int_0^d \sin\left(\frac{\pi z'}{d} \right) z' \sin\left(\frac{4\pi z'}{d} \right)$$

$$= \frac{2}{d} \left. \frac{d\left(25d \cos\left(\frac{3\pi z}{d} \right) - 9d \cos\left(\frac{5\pi z}{d} \right) + 120\pi z \sin\left(\frac{\pi z}{d} \right)^3 \left(2 + 3\cos\left(\frac{2\pi z}{d} \right) 157 \right) \right)}{450\pi^2} \right|_0^d = -\frac{32}{225\pi^2} d$$

$$\left(\frac{M_{1\to 4}}{M_{1\to 2}} \right)^2 = \left(\frac{32 \cdot 9}{225 \cdot 16} \right)^2 = \frac{1}{156}$$

$$E_{1\to 2} = \frac{\hbar^2}{2m^*} \frac{\pi^2}{d^2} (1 - 4) \Rightarrow \lambda_{1\to 2} = 29\mu m$$

NB: I did the integrals in Mathematica.

7. **Optical absorption of semiconductors in a magnetic field**
   (a) Using the result from question 1 above draw a sketch of the frequency dependence of the optical absorption of a one-dimensional direct gap semiconductor.

$$\rho(\varepsilon) = 2\sqrt{\frac{2m}{\varepsilon h^2}}$$

Diverges at the threshold for absorption.

   (b) Explain why a bulk semiconductor in a strong magnetic field can be considered as a one-dimensional system. Hence explain the shape of the optical transmission spectrum of germanium at 300K and 3.6T, shown in the figure below.

A strong magnetic field quantizes the motion in 2D perpendicular to the magnetic field, so the semiconductor becomes effectively 1-dimensional.

Electron Landau level : $E_n^e(k_z) = E_g + \left(n + \frac{1}{2}\right)\frac{e\hbar B}{m_e^*} + \frac{\hbar^2 k_z^2}{2m_e^*}$

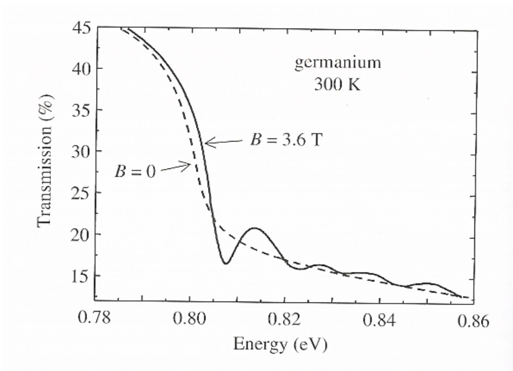
Hole Landau level : $E_{n'}^h(k_z) = -\left(n' + \frac{1}{2}\right)\frac{e\hbar B}{m_h^*} - \frac{\hbar^2 k_z^2}{2m_h^*}$

Photon transition energy : $\hbar\omega = E_g + \left(n + \frac{1}{2}\right)\frac{e\hbar B}{\mu} + \frac{\hbar^2 k_z^2}{2\mu}$

Absorption coefficient : $\alpha \propto (\hbar\omega - E_n)^{-1/2}$ $\quad E_n = E_g + \left(n + \frac{1}{2}\right)\frac{e\hbar B}{\mu}$

The divergence leads to dips in the reflectivity whenever the frequency becomes larger than the threshold for the next value of n.

(c) Use the data in the figure below to deduce values for the band gap and the electron effective mass of Ge based on the assumption that $m_h^* >> m_e^*$. Comment on which point of the Brillouin zone these values correspond to.

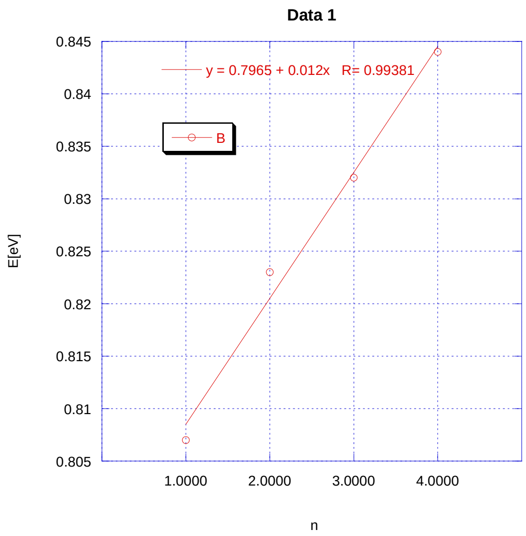


Absorption spectrum of Ge at 300K in a strong magnetic field, and without magnetic field.

(Hint: Remember from last year's course that the energies of electrons and holes in a parabolic band are quantized into Landau levels, and deduce from this the optical absorption between a specific Landau level in the conduction band E_n^{CB}, and the valence band E_m^{VB}. Assume a selection rule n = m between Landau levels.)

* NB: This question you will probably find more challenging than the others, but please give it a go, it is quite interesting.

E_1=0.807 eV
E_2=0.823 eV
E_3=0.832 eV
E_4=0.844 eV



E_g = 0.7965 eV

$m_e^*=\hbar B/0.012=0.035\ m_e$

These correspond to the Γ point of the Brilluoin zone.

8. k·p theory

- Conduction band energy higher than valence band energy; negative terms from conduction band change sign of effective mass, “CB repels VB”

- In cubic crystal symmetry of periodic part of Bloch wavefunctions is such that mass is isotropic; however in crystal with lower symmetry, such as orthorhombic crystals the vector product in the above expression between k and the matrix element of p is generally different in different directions, which gives rise to anisotropy.

- Joint density of states is the number of states that meet the energy conservation condition for vertical optical transition induced by photons with energy between ω and ω+dω. Dominates energy dependence of absorption if k-dependence of transition dipole matrix element is weak.

- Van Hove singularities arise when energy conservation condition for vertical transitions is satisfied between two parallel bands, i.e. $\vec{\nabla}_{\vec{k}}\left(E_c\left(\vec{k}\right)-E_v\left(\vec{k}\right)\right)=0$.

$$\hbar\omega = E_g + \frac{\hbar^2 k_x^2}{2m_{11}} + \frac{\hbar^2 k_y^2}{2m_{22}} + \frac{\hbar^2 k_z^2}{2m_{33}} + \frac{\hbar^2 k_x^2}{2m_e^*} + \frac{\hbar^2 k_y^2}{2m_e^*} + \frac{\hbar^2 k_z^2}{2m_e^*}$$

$$\hbar\omega - E_g = \frac{\hbar^2 k_x^2}{2m_1^*} + \frac{\hbar^2 k_y^2}{2m_2^*} + \frac{\hbar^2 k_z^2}{2m_3^*}$$

$$1 = \frac{\hbar^2 k_x^2}{2m_1^*\left(\hbar\omega - E_g\right)} + \frac{\hbar^2 k_y^2}{2m_2^*\left(\hbar\omega - E_g\right)} + \frac{\hbar^2 k_z^2}{2m_3^*\left(\hbar\omega - E_g\right)}$$

$$\frac{1}{m_i^*} = \frac{1}{m_{ii}} + \frac{1}{m_e^*}$$

Surfaces over which the energy conservation condition is fulfilled is an ellipsoid.
Problem is analogous to that of density of states.
Integral over the joint density of states is equal to total number of states, which is proportional to volume of ellipsoid.

$$\int \mathrm{J}_{\mathrm{cv}}\left(\omega'\right)d\omega' = 2\cdot\frac{1}{\left(2\pi\right)^3}\frac{4\pi}{3}\sqrt{\frac{2m_1^*\left(\hbar\omega - E_g\right)}{\hbar^2}}\sqrt{\frac{2m_2^*\left(\hbar\omega - E_g\right)}{\hbar^2}}\sqrt{\frac{2m_3^*\left(\hbar\omega - E_g\right)}{\hbar^2}} = N\left(\omega\right)$$

$$\frac{dN\left(\omega\right)}{d\omega} = \frac{1}{3\pi^2}\frac{3}{2}\left(\frac{2}{\hbar^2}\right)^{3/2}\sqrt{m_1^* m_2^* m_3^*}\sqrt{\hbar\omega - E_g} = \frac{1}{2\pi^2}\left(\frac{2}{\hbar^2}\right)^{3/2}\sqrt{m_1^* m_2^* m_3^*}\sqrt{\hbar\omega - E_g}$$