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EKSAMEN I FAG 74435 - FASTE STOFFERS FYSIKK 2
Fakultet for fysikk, informatikk og matematikk
Onsdag 12. januar 2000
Tid: 0900-1500

Tillatte hjelpemidler: B2 - Typegodkjent kalkulator, med tomt minne
O.Jahren og K.J. Knutsen: Formelsamling i matematikk
K. Rottmann: Matematische Formelsammlung/Matematisk formelsamling
S. Barrett og T.M. Cronin: Mathematical Formulae

SOLVE PROBLEMS 1, 2, 3 AND EITHER PROBLEM 4 OR 5

Problem 1

a) We shall study the electronic bandstructure $E(\overline{k})$ near a Bragg-plane. It is advantageous to write the $\overline{k}$-vector as $\overline{k} = \frac{1}{2}\overline{G} - \overline{q}$ where $\overline{q}$ measures the distance from the centre of a Bragg plane limiting the Brillouin zone. In terms of $\overline{G}$ and $\overline{q}$ the energy (a solution of the central equation) can be written in the form

$$E = E^o_{G/2} + \frac{\hbar^2 q^2}{2m} \pm \sqrt{4E^o_{G/2} \cdot \frac{\hbar^2 q_{||}^2}{2m} + |U_G|^2}$$

where $E^o_{G/2} = \frac{\hbar^2}{2m}\left(\frac{G}{2}\right)^2$. U_G is the Fourier coefficient of the potential and $q_{||}$ is the component of $\overline{q}$ parallel to $\overline{G}$. Assume that the Fermi energy has the value $E_F = E^o_{G/2} - |U_G| + \Delta$.

Show that when $0 < \Delta < 2|U_G|$ the Fermi surface will be lying entirely in the first Brillouin zone and cuts the Bragg-plane in a circle of radius

$$\rho = \sqrt{\frac{2m\Delta}{\hbar^2}}$$

b) Find the effective masses $m_{||}$ and $m_{\perp}$ parallel and normal to $\overline{G}$ in both bands near the zone boundary.

c) Use the effective mass approximation for the energies in the two bands and calculate the density of states in each band near the zone boundary.

Problem 2

a) At low temperatures and strong magnetic fields the magnetic susceptibility oscillates as the magnetic field is varied. This is called the deHaas - vanAlphen effect. Show that these periodic oscillations are given by the equation

$$\Delta\left(\frac{1}{B}\right) = \frac{2\pi e}{\hbar A_k}$$

where A_k is a cross-sectional area of the Fermi surface $\perp$ the magnetic field. Explain the concept and importance of the so called "extremal orbits".

b) The deHaas – vanAlphen oscillations in Cu for the socalled "belly orbits" (see Figure 1) have experimentally a period in 1/B equal to $1.83 \cdot 10^{-5}\ T^{-1}$. Determine the cross sectional area of the Fermi surface corresponding to these oscillations. Suppose now that Cu is a free-electron metal and calculate the cross-sectional area of the Fermi sphere. The density of Cu is $n = 8.45 \cdot 10^{28}\ m^{-3}$. Cu is monovalent. Compare the two areas and comment on the result. In the free electron model the Fermi energy is given by
$E_F = \frac{\hbar^2}{2m}\left(3\pi^2 n\right)^{2/3}$.

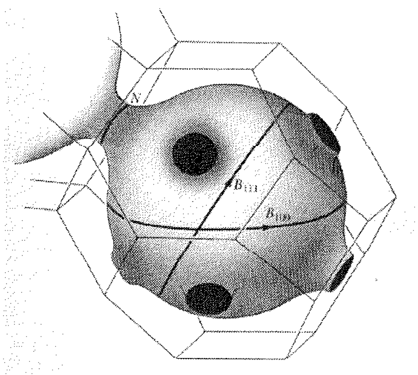

Figure 1

c) The crystal structure of Cu is face centred cubic. If we again assume that Cu is free electron like, we find that the Fermi sphere is lying entirely within the first Brillouin zone. Show that the Fermi surface will touch the Brillouin zone at the point $\frac{2\pi}{a}$(½, ½, ½) for an average charge of 1,36 electron/atom. This is the point on the Brillouin zone with the smallest distance from the centre of the zone.

Problem 3

We shall in this problem study a system which approximately behaves like a two-dimensional (2D) electron gas. Consider a non-interacting electron gas in a potential

$V=0$ for $|z|<\frac{d}{2}$ og $V=V_0$ for $|z|>\frac{d}{2}$ where d = 10nm. $V_0 \approx \infty$. The electrons can move freely in the x and y directions.

a) Show that the energy of the electrons is given by the expression

$$E(n,k)=f(d)\cdot n^2+\frac{\hbar^2}{2m}(k_x{}^2+k_y{}^2)$$

and determine f(d). Sketch E(n,k).

b) Calculate the density of states D(E) as a function of E.

Hint: For each value of n the system behaves like a two-dimensional electron gas. Calculate the density of states for each n and add. Sketch D(E).

c) What is the maximum temperature we can have and still observe 2D quantum effects even for low n-values. What is the maximum value of d where we still observe 2D quantum effects for low n values if the temperature of the system is 15 mK?

Problem 4

a) Define the n-th moment of the imaginary part of the dielectric constant, ε_2, as

$$M_n=\int_0^\infty \varepsilon_2(\omega)\omega^n d\omega$$

Use the Kramers Kronig relations to show that M_1 is determined by the total charge density in the material and that $M_{-1}=\frac{\pi}{2}(\varepsilon_1(0)-1)$

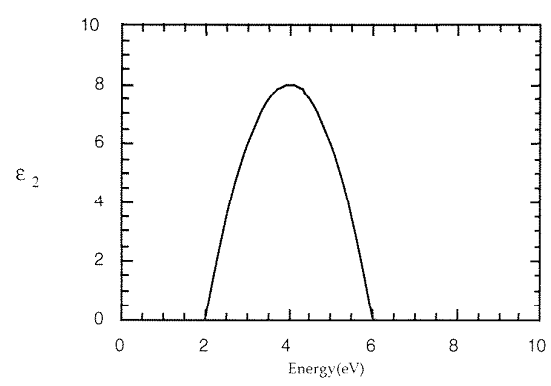

Figure 2

b) The figure shows ε_2 for a material with an absorption band between 2 and 6 eV given by: $\varepsilon_2 = -2(\hbar\omega - 2)(\hbar\omega - 6)$. $\varepsilon_2 = 0$ elsewhere. Use the Kramers Kronig relations to calculate:

i) $\varepsilon_1(0)$

ii) The plasma frequency for the material in electron volts and the electron density N.

Given:

Plasma frequency ω_p: $\omega_p^2 = \frac{Ne^2}{m\varepsilon_o}$

$$\hbar = 1.05 \cdot 10^{-34} \text{ Js}$$

$$m = 9.11 \cdot 10^{-31} \text{ kg}$$

$$\varepsilon_o = 8.85 \cdot 10^{-12} \text{ C}^2/\text{Nm}^2$$

$$e = 1.61 \cdot 10^{-19} \text{C}$$

$$\varepsilon_1 = 1 - \frac{\omega_p^{\ 2}}{\omega^2}$$

$$\varepsilon_1(\omega) = 1 + \frac{2}{\pi} P \int_0^\infty \frac{\xi \varepsilon_2(\xi)}{\xi^2 - \omega^2} d\xi$$

Problem 5

a) Give a brief account of the difference between the macroscopic field E in a crystal and the local field E_{loc} seen by an atom.

b) NaCl has a density $\rho = 2.17 \cdot 10^3$ kg/m^3 and a static dielectric constant $\varepsilon(0) = 5.9$. Using the Clausius-Mosotti equation, calculate the static polarisability $\alpha(0)$ of a NaCl ion pair. The molecular mass of NaCl is 58.4 g/mol. Calculate also the ratio $\frac{E_{loc}}{E}$. For visible light NaCl has a refractive index n = 1.54. Calculate the electronic polarisability $\alpha_{el}(\omega)$ for NaCl in this frequency range.

c) What dipole moment is induced in a NaCl ion pair when a NaCl crystal is placed in a static field with field strength $E_0 = 10^9$ V/m. How large displacement of the negative charges with respect to the positive does this represent?

Hint: Start with the equation $P = \chi E = (\varepsilon - 1)\varepsilon_o E$ and assume that the sample has a form where the macroscopic field E is equal to the external field E_0.

Given: Clausius Mosottis equation:

$$\frac{\varepsilon - 1}{\varepsilon + 2} = \frac{1}{3} N\alpha$$

Avogadros number $N_A = 6.02 \cdot 10^{23}$ mol^{-1}