Semiconductors and electron bands

Fall semester 2016, 04.01.2016, 13:45-16:30

Please note:

- There are 5 problems.
- The numbers of points per sub-problem are indicated on the right.
- There are some fundamental constants and a periodic table on back of this sheet.
- Please write clearly and readably. Try to be concise.
- Don't just write the final answer, also include the steps you took to get there.
- If we ask for a sketch, make sure that it clearly includes the qualitative features of the matter at hand, and label the axes.
- Write down your name and student number below (we'll staple all papers together in the end), and write your last name on each piece of paper.

Name:	Student number:

Problem	1	2	3	4	5	Total
Points						

List of physical constants

Atomic mass unit, 1 atm.u.	1.66×10^{-27} kg
Speed of light, c	3.00×10^{8} m/s
Planck constant, h	6.63×10^{-34} Js
$\hbar = h/(2\pi)$	1.05×10^{-34} Js
Electron charge, e	1.60×10^{-19} C
Electron volt, eV	1.60×10^{-19} J
Elektron masse, m_e	9.11×10^{-31} kg
Neutron masse, m_n	1.67×10^{-27} kg
Proton asse, m_n	1.67×10^{-27} kg
Vacuum permittivity, ϵ_0	8.85×10^{-12} As/Vm
Boltzmann constant, k_B	1.38×10^{-23} J/K
Rydberg constant, R_∞	1.10×10^{7} 1/m
Rydberg energy, hcR_∞	13.6 eV
Bohr magneton, μ_B	9.27×10^{-24} J/T
Bohr radius, a_0	5.3×10^{-11} m
Stefan-Boltzmann constant, σ	5.67×10^{-8} W/m^{2}K^4

1 H 1.00794																1 H 1.00794	2 He 4.002602
3 Li 6.941	4 Be 9.012182											5 B 10.811	6 C 12.0107	7 N 14.00674	8 O 15.9994	9 F 18.9984032	10 Ne 20.1797
11 Na 22.989770	12 Mg 24.3050											13 Al 26.581538	14 Si 28.0855	15 P 30.973761	16 S 32.066	17 Cl 35.4527	18 Ar 39.948
19 K 39.0983	20 Ca 40.078	21 Sc 44.955910	22 Ti 47.867	23 V 50.9415	24 Cr 51.9961	25 Mn 54.938049	26 Fe 55.845	27 Co 58.933200	28 Ni 58.6534	29 Cu 63.545	30 Zn 65.39	31 Ga 69.723	32 Ge 72.61	33 As 74.92160	34 Se 78.96	35 Br 79.504	36 Kr 83.80
37 Rb 85.4678	38 Sr 87.62	39 Y 88.90585	40 Zr 91.224	41 Nb 92.90638	42 Mo 95.94	43 Tc (98)	44 Ru 101.07	45 Rh 102.90550	46 Pd 106.42	47 Ag 196.56655	48 Cd 112.411	49 In 114.818	50 Sn 118.710	51 Sb 121.760	52 Te 127.60	53 I 126.90447	54 Xe 131.29
55 Cs 132.90545	56 Ba 137.327	57 La 138.9055	72 Hf 178.49	73 Ta 180.94.79	74 W 183.84	75 Re 186.207	76 Os 190.23	77 Ir 192.217	78 Pt 195.078	79 Au 196.56655	80 Hg 200.59	81 Tl 204.3833	82 Pb 207.2	83 Bi 208.58038	84 Po (209)	85 At (210)	86 Rn (222)
87 Fr (223)	88 Ra (226)	89 Ac (227)	104 Rf (261)	105 Db (262)	106 Sg (263)	107 Bh (262)	108 Hs (265)	109 Mt (266)	110 (269)	111 (272)	112 (277)		114 (289) (287)		116 (289)		118 (293)

58 Ce 140.116	59 Pr 140.50765	60 Nd 144.24	61 Pm (145)	62 Sm 150.36	63 Eu 151.964	64 Gd 157.25	65 Tb 158.92534	66 Dy 162.50	67 Ho 164.93032	68 Er 167.26	69 Tm 168.93421	70 Yb 173.04	71 Lu 174.967
90 Th 232.0381	91 Pa 231.035888	92 U 238.0289	93 Np (237)	94 Pu (244)	95 Am (243)	96 Cm (247)	97 Bk (247)	98 Cf (251)	99 Es (252)	100 Fm (257)	101 Md (258)	102 No (259)	103 Lr (262)

1 Short questions

a) Sketch the bandstructures for a semiconductor, an insulator, and a metal. Indicate the band filling. [3]

b) Assume a monoatomic tight-binding chain. Assume it is divalent, i.e. two electron per site. It it a metal, insulator, or semiconductor? Explain why. [3]

c) Give an intuitive argument as to why superconductors have a finite (i.e. larger than zero) coherence length. [2]

d) Sketch the dispersion relations of the electrons in a one-dimensional chain, both for solution using the tight-binding approximation, and for the solution using the nearly-free electron approximation.

e) Imagine a the surface of a superconductor, and a magnetic field outside the superconductor, parallel to the surface. Sketch the superfluid density and the magnetic field at the surface as a function of z, where z is the coordinate perpendicular to the surface. Make the sketch first for a type I and then for a type II superconductor. [3]

f) In a diatomic chain with N identical particles connected by springs, how many vibrational normal modes are there? Give a brief argument. [2]

2 1D monatomic chain with springs

Assume a chain with N identical atoms of mass m connected with springs with spring constant κ. In equilibrium, the atoms are spaced by distance a. Also assume that the atoms can only move along the chain, and not perpendicular to it (longitudinal modes).

a) Derive and sketch the dispersion relation. [3]

b) Show that the mode with wave vector k has the same physical meaning as the mode with wave vector $k + 2\pi/a$. (Make an explicit calculation if necessary.) [3]

c) Derive the number of different normal modes in the chain. [2]

d) What is the density of states $g(\omega)$? (Explicitly calculate it.) Sketch the density of states. Also sketch the density of states for a diatomic chain (you do not have to explicitly calculate it). [3]

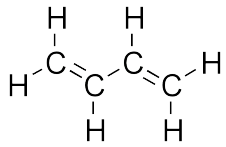
e) Find an expression for the specific heat of the chain in the limit of high temperatures compared to the phonon energies. You can assume that the the occupation numbers are governed by Bose-Einstein statistics,

$$f_{BE}(E) = \frac{1}{e^{\frac{E}{k_B T}} - 1}.$$

[3]

3 4-atom long tight-binding 'chain'

We look at a 4 atom long tight-binding chain. This is quite a good approximation for some molecules, like 1,3-butadiene (see image below). We ignore the hydrogen atoms and assume that only the carbon atoms are relevant. We denote them with the index n, $n = 1, 2, 3, 4$. They each have one electron in the outermost electronic shell. The Hamiltonian for the atom at site n (ignoring the other atoms) is $\mathcal{H}_n = T + V_n$, where T is the standard kinetic part, and V_n is the Coulomb potential from the ion at site n. We denote the solution to the Schrödinger equation at site n (ignoring the other atoms) with $|n\rangle$, i.e. $\mathcal{H}_n|n\rangle = E|n\rangle$.



a) What is the full Hamiltonian $\mathcal{H}_{\text{total}}$ for one electron on the chain? (Ignore any electron-electron interaction.) [2]

b) We assume that there is only nearest neighbour interaction and define $t = \langle n|\mathcal{H}_{\text{total}}|m\rangle$ when n, m are nearest neighbours. We also assume that the orbital functions are orthogonal. Using the Ansatz $\Psi = \sum_{n=1}^{4} \phi_n|n\rangle$, derive the Schrödinger equation in Matrix form. Explicitly write down the matrix equation. Show that the solution of this equation is the ground state by minimizing the energy functional. [5]

c) How would you solve this to get the energy eigenvalues and eigenfunctions? (You don't have to do the calculation.) [1]

d) Guess how the absolute value of the wave function of the lowest energy state looks like in real space and sketch it. Briefly argue why it should look like that. [2]

e) Describe in words what happens to these energy states when you increase the number of atoms and how you get to the limit of the tight-binding chain (roughly three sentences). [3]

4 Width of the depletion layer

Calculate the width of the depletion layer in a pn junction. We assume that the interface of n and p doped semiconductors is at $x = 0$, and perpendicular to the x axis, with the n doped one on the negative side. he junction consists of two same semiconductors with gap E_g and electron doping with concentration n on one side, and hole doping with concentration p on the other side. We also assume that we are at temperatures much smaller than the bandgap, but above the carrier freeze-out.
Let $\phi(x)$ be the potential which reflects the bending of the bands, and ϕ_0 the potential difference across the junction with no applied voltage. We refer to the width of the depletion layer on the two sides as w_n and w_p. T Inside the depletion layer, all the electrons and holes recombine, while outside, none do.

a) Remember Poisson's equation:

$$\frac{\partial^2}{\partial x^2}\phi(x) = \frac{\rho(x)}{\varepsilon_0 \varepsilon_r},$$

where $\rho(x)$ is the charge density, ε_0 is the vacuum permittivity, and ε_r is the relative permittivity. Based on the simple picture for a pn junction from the lecture, make assumptions for the charge density and write down the Poisson equation. [3]

b) Solve them to get allow expressions for $\phi(x)$ on the negative and positive side. (Set $\phi(x) = 0$ for $x = 0$.) You will have integration constants in these expressions. [3]

c) Obtain the integration constants form boundary conditions. [3]

d) Find an expression for w_n and w_p. [2]

5 Magnetism in a gas

Consider a gas of monovalent atoms with spin 1/2, and $L = 0$ in a magnetic field B. The density of the gas is n. The g-factor is 2.

a) What would be an example for such a gas? [2]

b) Calculate the magnetisation as a function of B and T. Determine the susceptibility. [3]

c) Calculate the contribution to the specific heat of this gas due to the spins. Sketch this contribution as a function of $\mu_B B/k_B T$. [4]

END OF EXAM