The electronic structure of solids

Fall semester 2017, 08.01.2017, 14:00-17:00

Please note:

- There are 4 problems.
- The numbers of points per sub-problem are indicated on the right.
- There are some fundamental constants and the 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	Total
Points					

List of physical constants

Atomic mass unit, 1 atm.u.	$1.66{\times}10^{-27}$ 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
Electron mass, m_e	9.11×10^{-31} kg
Neutron mass, m_n	1.67×10^{-27} kg
Proton mass, 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 110.710	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

Please answer with a sketch and/or a short (roughly two sentences) text.

a) Sketch the band structures for a semiconductor, an insulator, and a metal. Indicate the band filling and indicate typical values for the band gaps, if applicable. [3]

b) Sketch the electronic dispersion relations of the electrons in a one-dimensional chain for the nearly-free electron approximation in the extended zone scheme, with the atomic potential being a cosine function. Draw the lowest three bands. [3]

c) Remember the classic experiment of a small magnet levitating above a high-temperature superconductor immersed in liquid nitrogen. Explain briefly why one can observe this phenomenon. [3]

d) Draw the dispersion relation for phonons in a diatomic chain. Which phonons (mark them in the sketch) couple to photons and why? [4]

e) Explain which phenomena determine the width of the depletion layer. [3]

f) Which spin-spin interaction leads to the formation of domains in a piece of iron? [3]

2 One-dimensional Morse solid

Assume a chain with N identical atoms of mass m. Nearest neighbor atoms are coupled by the so-called Morse potential

$$V_M(r) = D\big(1 - e^{-\alpha(r-r_0)}\big)^2 - D$$

where r is the distance between them and D, α, and r_0 are positive parameters.

a) Calculate $V_M(0)$, $V_M(r_0)$, $V_M(\infty)$ and qualitatively sketch the Morse potential. [3]

b) Find the equilibrium distance between the atoms at zero temperature. [3]

c) Determine the harmonic approximation to the total potential energy $V = \sum_j V_M(x_{j+1} - x_j)$ by expanding to quadratic order in the displacements δx_j from the rest positions. [3]

d) Write down the classical equations of motion for the displacements in harmonic approximation. [3]

e) Calculate the dispersion relation of the phonons, assuming periodic boundary conditions. [3]

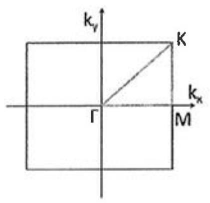
f) Calculate the speed of sound in terms of the potential parameters given above. [3]

3 Tight Binding in 2D

Consider a rectangular lattice in two dimensions, with lattice constants a_x and a_y. Now imagine a tight binding model, where the hopping matrix element is $\langle n|H|m\rangle = t_1$ if sites n and m are neighbors in the horizontal direction and $\langle n|H|m\rangle = t_2$ if n and m are neighbors in the vertical direction.

a) First, assume that there is one orbital at each lattice site. Calculate the dispersion relation for this tight binding model and show that it is of the form $E = \varepsilon - 2t_1\cos(k_x a_x) - 2t_2\cos(k_y a_y)$. [4]

b) Sketch the dispersion in a graph with three adjacent panels, E on the vertical axis, k along the three high-symmetry directions, i.e. along paths $\Gamma M, MK, K\Gamma$. [3]



c) Now assume two orbitals α, β per lattice site, with atomic energies $\epsilon_\alpha = 3\text{eV}$ and $\epsilon_\beta = 10\text{eV}$. Assume further $t_1 = 1\text{eV}$ and $t_2 = 0.5\text{eV}$ for both orbitals. Argue why this is a semiconductor if there are 2 electrons per site. [4]

d) Calculate the direction dependent band mass for holes. [4]

4 Magnetism

a) Derive the magnetic susceptibility for an electron gas (Pauli paramagnetism). [4]

b) Why is the susceptibility in Pauli paramagnetism at low temperatures much smaller than the susceptibility in Curie paramagnetism of atoms? [3]

c) We now turn on interactions between electrons. Write down the interaction term of the Hubbard Hamiltonian with parameter U (Hubbard interaction parameter). Considering for the kinetic part a hopping parameter t (e.g. from tight binding), explain why for half filling the Hubbard model describes an insulator for $t \ll U$. [4]

d) Estimate the energy gain from the Hubbard interaction term as a function of magnetization M. *Hint:* Remember $4ab = (a+b)^2 - (a-b)^2$ for any $a, b \in \mathbb{C}$ and use mean-field like approximation. [4]

END OF EXAM