FRIEDRICH-SCHILLER-UNIVERSITÄT JENA
Institute of Condensed Matter Theory and Solid State Optics – PAF
Stefan Skupin
Oleg Egorov, Dörte Hansen

WS 2013/2014

Exam
STRUCTURE OF MATTER

February 21

Exercise 1

2+3+3 Points

Please answer the following questions shortly.

a) Explain the implication of the Kramers-Kronig relations with respect to the physical effects related to real and imaginary part of the complex dielectric function $\epsilon(\omega)$.

b) Consider the simplest model of Hydrogen atom, disregarding relativistic and spinor effects. Please sketch the spectrum of the Hydrogen atom. How do the energy eigenvalues depend on the quantum numbers?

c) Please sketch the spectrum of an one-dimensional quantum mechanical harmonic oscillator. How do the energy eigenvalues depend on the quantum number? Discuss the ground state of the quantum mechanical harmonic oscillator.

Exercise 2

2+3+6 Points

Consider a typical glass with a dielectric function which is characterized by two Lorentz-type resonances:

$$\epsilon(\omega) = 1 + \frac{f_p}{\omega_p^2 - \omega^2 - ig_p\omega} + \frac{f_e}{\omega_e^2 - \omega^2 - ig_e\omega}.$$

a) Please explain the origin of both resonances and give their typical orders of magnitude. Explain the physical meaning of all parameters.

b) Sketch real and imaginary part of $\epsilon(\omega)$. Mark the frequency ranges with strong absorption, normal and anomalous dispersion.

c) Let us assume that the losses are negligible ($g_p = 0$, $g_e = 0$). Show that the dielectric function in the optical frequency domain ($\lambda_e \ll \lambda \ll \lambda_p$) can be written in good approximation as

$$\epsilon(\lambda) \simeq A - B\lambda^2 + \frac{C}{\lambda^2} + \frac{D}{\lambda^4}.$$

Determine the empirical coefficients A, B, C, D as functions of the model parameters f_p, f_e and $\lambda_p = 2\pi c/\omega_p$, $\lambda_e = 2\pi c/\omega_e$.

Exercise 3

1+3+3+4 Points

The vibrational and rotational degrees of freedom of molecules contribute to the energy spectrum in addition to its pure electronic transitions.

a) What are typical frequency ranges of purely rotational and purely vibrational spectra?

b) Explain the main idea of Frank-Condon principle for a diatomic molecule with only one vibrational degree of freedom.

c) Sketch the excitation and de-excitation of that molecule, using an energy configuration diagram of the molecule in the electronic ground state and in an excited state.

d) Sketch the typical emission and absorption spectra of the optical transitions between the electronic ground state and an excited state of the molecule, taking into account the vibrational degree of freedom. Please give some short explanations. How is the center frequency ω_0 defined?

Exercise 4 **2+6+3 Points**

Lattices are periodic arrangements of points and provide the mathematical tool for treating crystalline structures. The most important lattices have been introduced by Bravais in the 19th century already.

a) Sketch the body centered cubic (bcc) and face centered cubic (fcc) Bravais lattices. What is a primitive cell of a Bravais lattice? What is a Wigner Seitz cell?

b) Consider a primitive cell, whose basis vectors are given by

$$\mathbf{a}_1 = \frac{a}{2}(1,0,1),\ \mathbf{a}_2 = \frac{a}{2}(0,1,1),\ \mathbf{a}_3 = \frac{a}{2}(1,1,0).$$

Which Bravais lattice can be related to this? Calculate the corresponding reciprocal lattice and identify, which type of Bravais it represents.

c) Quantum mechanical wavefunctions of electrons in a periodical potential satisfy the general statements known as Bloch's theorem. Please formulate Bloch's theorem and explain its meaning.

Exercise 5 **2+2+3+7* Points**

Many essential properties of the energy spectrum of a crystal can be understood by using the Kronig-Penney model for an electron in a one-dimensional periodic potential. In the simplest case, this potential is given by a periodic arrangement of δ-like atoms,

$$V(x) = V_0 \sum_{n=-\infty}^{\infty} \delta(x - na),$$

where a is the lattice constant and $V_0 > 0$.

a) Show, that the first derivative of the electron wavefunction $\psi(x)$ jumps at $x = na$ according to

$$\psi'(na + \varepsilon) - \psi'(na - \varepsilon) = \frac{2mV_0}{\hbar^2}\psi(na).$$

Here $\varepsilon \to 0$ and m is the electron mass and n is an integer number.

b) Solving the Schrödinger equation, find a general solution for an electron of energy E in the regions between δ-potentials, i.e. $(n-1)a < x < na$.

c) For the given potential, one finds the following relation between the Bloch's vector k_B and $k = \sqrt{2mE/\hbar^2}$:

$$\frac{mV_0 a}{\hbar^2}\frac{\sin ka}{ka} + \cos ka = \cos k_B a. \qquad (1)$$

Sketch the graphical solution and explain the origin of the gaps and allowed energy bands.

d)* Now assume that the strength of the potential is large, i.e. $P = mV_0 a/\hbar^2 \gg 1$. Find an approximative solution $E(k_B)$ for that case.
Hint: Start from equ. (1) and consider a Taylor expansion around the first zero of $\frac{\sin ka}{ka}$.