YFX8020-Solid States Physics and Semiconductors Physics

List of questions for the first part of the final exam (take place at second half of March)

1. Crystals symmetry properties (p. 1-15, 31-55)[3]
Elements of points groups, rotations (C_n^k), reflection (σ), inversion (I), rotary-reflection(S_n^k). The examples of point groups (C_n, C_{nh}, D_{nh}, T, T_d, O_h). Translational symmetry. Basis vectors. Elementary cell. Volume of elementary cell. Simple and complex cells. Niggly theorem. Crystals classes. Bravais latices. Examples of simple structures (cubic simple, cubic volume and base centered lattices, NaCl, Diamond , Wurzite, CsCl, $BaTiO_3$) lattices. Direct and reciprocal lattices. Base vectors for reciprocal lattice (examples of calculation). Wigner-Zeits cell. Space goups.

2. X-ray (p. 15-21)[3]
The Laue and Bragg equations for X-Ray diffraction in Crystals. Atomic and structural scattering factors (explanation). Miller indices.

3. Vibrations of crystals.(p.171-181)[3]
3.1 One dimensional simple chain.(p. 111-117,171-181)[3]
Description of atomic vibration for simple 1-d linear (forces acting on each atom have a linear dependence on deflection of atoms from equilibrium position) lattice. Equation of motion for atoms. Solution of the system of the equations of motion (harmonic traveling wave). Dispersion relation. Density of vibrations. Total internal mechanical energy of lattice. Transition from classical to quantum-mechanical description of the total energy. Bose-Einstein distribution. Calculation of heat capacity. Compare with experiment and with classical approach.

3.2 One dimensional complex chain (two atoms in elementary cell). (p. 117-125,171-181)[3]
One dimensional complex (atoms per each elementary cell) lattice. Equation of motion for atoms. Dispersion relations. Optical and acoustic branches. Nature of atomic motion for q=0.

3.3 3d crystals. (p. 125-137,171-181)[3]
Expanding the interatomic potential energy into a power series. Calculation of the interatomic force constants. Equation of motion for atoms in 3d complex crystals. Solution of the equation of motion. Dynamical matrix. Diagonalisation. Dispersion relations, eigenvectors (vectors of polarization) and eigenvalues (frequencies of vibrations) . Density of vibrations. Example for CsCl, Nacl and $BaTiO_3$.

4. Chemical bonds (explanation of the nature of chemical bonds.) (p. 103-111)[3].

Examples and characteristic properties of materials (lattice structure; electronic, optical and elastics properties).

4.1 Ionic crystals.
4.2 *Covalent crystals.*
4.3 *Metals.*
4.4 *Van-der-Waals and hydrogen bonds.*

5. Addiabatic approximation(p. 190-193)[3]
Schredinger equation for crystal (Full Hamiltonian). Presentation of total wave-function. Use of the fact that the electron mass m_e is much less than the nuclear masses M (adiabatic approximation). Schredinger equations for nucleus and electrons. Separation the motion of electrons and nucleuses.

6. Hartree-Fock method.(p.193-200)[3]
The solution of the Schredinger equation for electrons. Total exact wave function for electrons. The presentation of this function as a multiplication of one-electron functions or by determinant (Pauli principle). Coulomb and exchange energies. Effective external field. Algorithm of Hartree-Fock calculations. The contribution of correlations. Method of pseudopotentials.

7. Gas of free electrons.
6.1 Schredinger equation for free electrons in **1d** lattice. Solution of equation, periodical boundary conditions, Fermi energy. Density of states. Fermi-Dirac distribution. Heat capacity for gas of free electrons.
6.2 Schredinger equation for free electrons in **3d** cubic lattice. Solution of Schredinger equation, periodical boundary conditions, Fermi energy. Density of states. Fermi-Dirac distribution. Heat capacity of gas of the free electrons. Brillouine zone. Bloch functions.

8. Almost free (weakly bonding) electrons or electrons in a weak periodical potential.(p. 204-219)[3]
Dependence of energy on the wave vector for electrons in 1d lattice. Property of periodicity for this dependency. Calculation of the electron band structure by perturbation theory (for weak periodical potential). The energy spectrum of almost free electrons. Bands structure and forbidden energy bands. The bandgap appearing.

9. Tight-Binding approximation(p. 224-234)[3]
Schredinger equation for isolated atoms and for high localized electrons in crystal. Formation of wave function. Calculation the electron energy. Band structure. Forbidden zone. Band gap. Effective mass calculation. Example for simple cubic lattice.

10.Additional questions

10.1 Anharmonicity, heat conductivity and thermal expantion. (p. 186-189)

10.2 LT-spliting(p.315-318, 323)[3]
Long-wave(q=0) vibrations in ionic crystals.Mechanism of LT-splitting (Effective electrical field). Ewald method for calculation the electrostatic energy. Ewald constant.

10.3 Excitons,Polarons(p. 163-167)[3]
Schredinger equation for excitons with large radius. Energy levels of excitons. Polaron (Explanation).

10.4 Effective masses of electrons (p. 204-207)[3]
Calculation of effective masses (examples). Approximation of effective masses.

Textbooks:

1. Ch. Kittel, "*Introduction to Solid State Physics*"
2. Ashcroft, N.W., Mermin, N.D. "*Solid State Physics*"
3. A. Anselm, "*Introduction to the theory of semiconductors*"