Class “Solid State Electronics + TCAD” — Academic Year 2010–2011 — March 01 through June 10, 2011

Presentation and aims of the course. Schedule. Notions that should already be known to the Students. Exams. Contents. References.
Analogy between the variational principles of Optics and Mechanics. Hypothesis of generalization of Mechanics. Planetary model of atoms and explanation of some atomic phenomena by means of such a model.

Experimental results not explained by the "classical" laws. Stability of atoms, spectral lines of excited atoms, photoelectric effect, black-body radiation. Planck's hypothesis, Planck's law. Einstein's theory of the photoelectric effect. Compton effect and its explanation using the hypothesis of the photon. Hall effect.
Davisson and Germer's experiment. Bohr's hypothesis. Quantization of the dynamical quantities. De Broglie's hypothesis. Wave function for the motion in free space. Contraction of the wave function. Perturbation induced by a measurement. Normalization of the wave function.

Schrödinger equation independent of time. Hamiltonian operator: definition and properties. Examples: free particle, particle confined within a one-dimensional box with infinite walls. Scalar product of functions. Hermitian operators. Properties of the eigenvalues and eigenfunctions of Hermitian operators. Completeness of a set of functions. Superposition of states. Deduction of the Schrödinger equation dependent on time. Norm conservation. Wave packet.

Introduction to the general methods of Quantum Mechanics. Successive measurements of position and momentum. Measurements of energy. Theorems about operators. Simultaneously observable quantities. Commutative operators. Examples.

Statistical concepts associated to quantum operators. Expectation value of an operator. Demonstration of the uncertainty principle. Minimum-uncertainty wave function. Time derivative of the expectation value. Ehrenfest theorem.

Examples of solution of the Schrödinger equation. Potential-energy step. Wave packet and limiting cases. Potential-energy barrier. Tunnel effect. Potential-energy well. Introduction to the problem of the linear harmonic oscillator. Importance of the problem. Calculation of the eigenvalues and eigenfunctions. Quantization of the energy and momentum of the electromagnetic field. Concept of photon.

Symmetrical or anti-symmetrical functions and operators. Systems made of identical particles. Fermions and bosons. Constructing symmetrical or anti-symmetrical wave functions basing upon the solution of the Schrödinger equation. Pauli exclusion principle. Statistical treatment of sets of identical particles. General concepts about the equilibrium statistics. Derivation of the Fermi-Dirac statistics. Classical limit of the F-D statistics. Stirling approximation. Derivation of the Bose-Einstein statistics. Calculation of the density of states for the e.m. field within a box. Derivation of the Planck law. Calculation of the Lagrange multiplier within the Planck law.

Time-dependent perturbation theory. Reduction to a set of differential equations in the coefficients of the expansion, transformation into an integral equation. Solution of the equations. Fermi's golden rule. Properties.

Lattice vibrations. Second-order expansion of the potential energy. Diagonalization of the elastic-coefficient matrix. Classical treatment of the small oscillations. Adiabatic approximation. Single-electron Hamiltonian.

Introduction to crystals. Direct lattice. Characteristic vectors. Translational vectors. Wigner-Seitz cell. Translational operators. Periodic operators. Bloch theorem and Bloch functions. Periodicity of the eigenvalues of the translational operators. Krönig-Penney model. Hint about the calculation of the dispersion relation in three dimensions. Definition of the effective-mass tensor.

Wave packets in a periodic potential. Symmetry of the eigenvalues. Energy bands. Example: silicon. Density of states in the phase space. Density of states in energy for a parabolic band. Form of the dispersion relation of the conduction and valence bands for Ge, Si, and GaAs. Distribution function. Density of states in the general case. Definition of hole concentration. Qualitative discussion about conductors, insulators, and semiconductors at equilibrium. Calculation of the intrinsic concentration. Fermi integrals and exponential approximation for them. Examples of the parameters determining the gap and intrinsic concentration in Ge, Si, and GaAs. Definition of the average velocity of electrons and holes. Comments.

Dynamics of an electron in a crystal. Equivalent Hamiltonian. Effective-mass theorem. Effect of the dopants. Band diagrams for an n-type semiconductor. Calculation of the extrinsic concentrations in the uniform case. The case of non degeneracy and complete ionization. Compensation effect. The non-uniform case. The Poisson equation.

Liouville theorem. Boltzmann transport equation (BTE). Relaxation time. Moments' method. Moment of order zero of the BTE. Physical meaning of the terms appearing in the moment of order zero. Moment of order 1 of the BTE. Simplifications and meaning of the terms appearing in the moment of order 1 of the BTE. Electron-temperature tensor. Electron-temperature tensor in the equilibrium case. Relaxation-time tensor. Moment of order 1 for a single valley. Current density for a single valley. Simplifications for the case of a low magnetic field. The simplified diffusive term. Mobility and diffusivity tensors.

Compensation of anisotropy when the perturbation with respect to equilibrium is small. Drift-diffusion transport equations including the magnetic field. Einstein relations. Mathematical model of semiconductor devices. Quasi-static approximation. Purely Ohmic equations including the magnetic field. Use of the Ohmic equations in the measurement technique based on the Hall effect. Hall voltage and Hall coefficient. Explanation of the atoms' stability.

TCAD practice: Generation of geometrical and physical structures for semiconductor-device modeling and simulation. Solution of the semiconductor-device model over the generated structures. Effects of changes in the microscopic parameters (e.g., lattice temperature). Practice on typical semiconductor devices.