

Module: Molecular Quantum Mechanics

WS 2011/12

Lecture: 3 SWS, Exercises 1 SWS

Exam: oral, graded

Contents with slide numbers

1	Mathematical Basis	7
1.1	Schrödinger's Equation	8
1.2	Operators and Observables	14
1.3	Fourier Transformation	28
2	Angular Momentum	34
2.1	Angular Momentum	35
2.2	Ascending and Descending Operators	43
2.3	Eigenfunctions of the Angular Momentum Operator	48
2.4	Spin	58
2.5	Addition of Angular Momenta	62
2.6	Rotation Spectra	75
3	Perturbation Theory	83
3.1	Time-Independent Perturbation Theory	85
3.2	Degenerate Energy Levels	100
3.3	Time-Dependent Perturbation Theory	104
3.4	WKB Method	119
4	Relativistic Methods in Quantum Chemistry	124
4.1	Special Relativity	126
4.2	Dirac Equation	133
4.3	One-Electron Atoms	140
4.4	Many-Particle Systems	142
5	Theory of the Solid State	154
5.1	Periodicity	156
5.2	Reciprocal Lattice	163
5.3	Vibrations in a One-Dimensional Chain (Dispersion Relation)	165
5.4	Free Electrons in the Solid State	178
5.5	Band Structures in the Solid State	190
5.6	Magnetism	210
5.7	Transport Phenomena, Conductivity	219

6 Density Functional Theory	231
6.1 Introduction	232
6.2 The Hohenberg–Kohn Theorems	239
6.3 The Kohn–Sham Method	246
6.4 Approximations to the Kohn–Sham Functional	265

List of Topics

1. Mathematical basis of quantum mechanics: Schrödinger’s equation, Hilbert space, bra-ket notation, operators and observables, Hermitian operators, expansion of wave functions, Dirac’s delta function, continuous spectra, representations, Fourier transformation
2. Angular momentum: commutator relations for \hat{L} and \hat{L}^2 , ascending and descending operators (shift operators), eigenvalue spectrum of the angular momentum, eigenfunctions – spherical harmonics, spin, addition of angular momenta, Clebsch-Gordan coefficients, rotation spectra - centrifugal potential
3. Perturbation theory (PT): approximate methods to solve Schrödinger’s equation, time-independent PT, intermediate normalization, orders of perturbation, first-order energy and wave function corrections, second-order corrections, PT for degenerate energy levels, time-dependent PT, interaction of radiation with matter, transition probabilities, transition dipole moments, selection rules, higher order time-dependent PT, WKB method
4. Relativistic methods in quantum chemistry: special relativity and Lorentz transformation, relativistic Hamiltonian, Dirac equation (relation to Schrödinger’s equation), Pauli equation, magnetic potential, relativistic solutions for one-electron atoms, Coulomb–Breit operator, relativistic corrections for many-particle systems, Dirac–Hartree–Fock
5. Theory of the solid state: periodicity, lattices, Fourier series, reciprocal space, one-dimensional chain, dispersion relation, optical and acoustic branches, Brillouin zone, free electrons in the solid state, density of states, Fermi gas, Fermi energy, Fermi statistics, band structures, Bloch theorem, periodic perturbations to the free electron, strongly bound electrons, interpretation of band structures, magnetism, origin of diamagnetism and paramagnetism, exchange interaction, exchange hole, ferromagnetism, conductivity, effective mass, particles and holes, superconductivity
6. Density functional theory (DFT): variational principle, electron density, Hohenberg–Kohn theorems, Levi’s proof of DFT, Kohn–Sham method, exchange-correlation energy, spin density functional theory, H_2 -dissociation: exchange and correlation holes, local density approximation, generalized gradient approximation, hybrid functionals, adiabatic connection, Jacob’s ladder