Module:
Molecular Quantum Mechanics

WS 2011/12

Lecture: 3 SWS, Exercises 1 SWS
Exam: oral, graded

Contents with slide numbers

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