

# AMO physics

Learning outcomes

# A for atoms

- Write the Schrödinger equation for the Hydrogen atom in terms of angular momentum
- Sketch and understand the effective potential of the hydrogen atom in terms of angular momentum
- Sketch and understand the radial and angular parts of the hydrogen atom orbitals
- Know lengths scales of the hydrogen atom, as a function of  $n$
- Know the hydrogen spectrum (Bohr formula), accidental and essential degeneracies for levels and orders of magnitudes
- Know the different corrections to the Hydrogen spectrum and their physical origin
- Understand their consequences on degeneracies and angular momentum of levels
- Estimate orders of magnitude for these effects
- Write the Schrödinger equation in the presence of external fields

# A for atoms

- Know what are the Zeeman and Stark effects, and calculate their first order contributions to the spectrum
- Understand the concept of vector operators, and how their matrix element are calculated
- Sketch the spectrum of the Helium atom
- Estimate the effects of Coulomb repulsion using variational methods and perturbation theory
- Write the direct and exchange interactions for two electrons, and their effect on the single and triplet states
- Sketch and understand the screened Coulomb potential for an atom with several electrons
- Understand the structure of the periodic table based on the independent electrons approximation and the central field approximation
- Know and understand the physics behind the different approximation techniques for atomic structures: central field, Thomas-Fermi, Hartree-Fock

# M for molecules

- derive and argue about the Born-Oppenheimer approximation
- perform the estimates of the relevant time and energy scales for electronic vibrational and rotational transitions
- know how to derive the potential energy surfaces of the H<sub>2</sub><sup>+</sup> molecule-ion
- know how to derive the Heitler-London model of chemical bonding in the H<sub>2</sub> molecule
- understand the ways of systematic improvement of the electronic structure models of molecules
- apply variational principle, derive and apply the Rayleigh-Ritz method
- understand the concept of basis sets and molecular orbital = linear combination of atomic orbitals (MO-LCAO)
- classification of molecular orbitals (bonding/antibonding/nonbonding, sigma/pi/.. )

# M for molecules

- understand the difference between core and valence atomic orbitals
- sketch the MO diagrams of diatomic molecules and use them to conclude on the bond order, spin state
- understand the concept of hybridization and relate it to the structure of molecules
- sketch the MO diagrams of diatomic molecules and use them to conclude on the bond order, spin state
- understand the concept of hybridization and relate it to the structure of molecules
- understand the approximation behind the Hückel model of pi-conjugated molecules
- perform the calculations using the Hückel model and represent graphically the results (MO diagrams, MOs)
- calculate the rotational and vibrational energy levels of diatomic molecules

# M for molecules

- know and understand the gross and specific selection rules for various types of molecular spectroscopy
- calculate parameters of diatomic molecules (interatomic distance, force constant, etc.) from molecular spectra
- reciprocally, draw molecular spectra given the necessary parameters
- understand the effects of centrifugal distortion and anharmonicity and be able to describe them using the respective parameters
- know the classification of rotors in the context of rotational spectroscopy
- calculate rotational spectra of molecules represented by symmetric rotors
- understand how to calculate vibrational spectra of polyatomic molecules
- calculate the number of vibrational modes of polyatomic molecules and be able to conclude about their IR activity
- explain the Franck-Condon principle and derive the Franck-Condon parameters

# O for Optics

- Write and understand the propagator in reciprocal space
- Represent a wave using angular spectrum
- Classify waves as propagating or evanescent
- Understand the paraxial approximation
- Understand the propagation of Gaussian beams
- Understand diffraction in the Fresnel (paraxial) and Fraunhofer conditions
- Use the paraxial propagator and the thin lens approximation to calculate the field in optical elements
- Understand the physical origin of the diffraction limit to optical resolution
- Write the light-matter interaction Hamiltonian in the long-wavelength approximation
- Understand the dipole selection rules
- Understand and explain the notions of absorption, stimulated and spontaneous emission
- Use perturbation theory to estimate stimulated emission and absorption probabilities

# O for Optics

- Solve the Schrödinger equation for a two-level atom in an external field
- Sketch and understand Rabi oscillations, and their relations to absorption and emission of light
- Understand and sketch the probabilities of ground and excited states as a function of frequency and amplitude of the field
- Write simple rate equations for atomic populations in the presence of injection and losses
- Sketch the populations of ground and excited states atoms a function of frequency and amplitude of the field
- Connect the electron wave function obtained from Schrödinger equation with the macroscopic polarization
- Sketch and understand the real and imaginary parts of the index of refraction as a function of parameters
- Understand the gain mechanism and operation of lasers

## E for Exam

- 4 to 5 small exercises (smaller than problems in exercise sheets)
- Covering widely the topics of the course
- 1/3 knowledge and understanding of concepts
- 2/3 small calculations