Concepts of Quantum Mechanics (iMOS)

Module	Credits	Workload	Term	Frequency	Duration
1 EC	5 CP	150 h	1 Semester	Each WiS	1 Semester
Courses a) Lectures b) Exercises			**Contact hours** a) 2 SWS b) 2 SWS	**Self-Study** 90 h	**Group size** 10-20 Students

Prerequisites

Knowledge of the following principles: Mathematics (Differential calculus, Integral calculus and Calculus of variations, Real and complex functions)
Basic principles of probability theory
Elementary quantum mechanics (harmonic oscillator, spin)

Learning outcomes

After completion of this course, students will know selected concepts and techniques of quantum mechanics and quantum statistical mechanics suitable to describe (bio)molecular systems such as molecules, clusters, liquids, solids and surfaces at an advanced level. They will be skilled in assessing which tool is suited to address a given question concerning dynamics and simulation, electronic and molecular structure, and theoretical spectroscopy of the aforementioned systems, and able to select relevant techniques and apply them to the quantum mechanical assessment of (bio)molecular systems.

Content

Introduction to quantum mechanics: postulates of quantum mechanics, Schrödinger equation, uncertainty principle (2h)

Review of basic quantum mechanics: real-space and momentum-space representation, bra/ket formalism and connection to the vector space and completeness relation (2h)

Free particle, particle in a box (1D and 2D) (2h)

Harmonic oscillator: algebraic solution, ladder operators (2h)

Central potentials: the Hydrogen atom (2h)

Pauli principle and antisymmetrization of wavefunction, spin and orbital angular momenta (4h)

Non-degenerate time-independent perturbation theory, variational principle (Rayleigh-Ritz), Hartree Fock (4h)

Time-dependent quantum mechanics: Schrödinger, Heisenberg and Dirac picture, time-dependent Schrödinger equation, Heisenberg equation of motion, time evolution operator (4h)

Time-dependent perturbation theory: intermediate/interaction picture, transition probabilities, constant and periodic perturbations, sudden approximation (4h)

Introduction to quantum-statistical mechanics: statistical/density operator, thermal density matrices, quantum-statistical expectation values, statistical mixtures and pure states, thermal Boltzmann operator (2h)

Teaching methods

Lectures and exercises with active participation during lectures, weekly homework corrected by teaching assistant and/or interactive presentation of homework during exercises

Mode of assessment

30-45 min end-of-term oral exam or 2-hour end-of-term written exam

Requirement for the award of credit points

Passing the oral or written examination
Module applicability M.Sc. iMOS
Weight of the mark for the final score According to CP
Module coordinator and lecturer(s) Prof. Dr. Sulpizi lecturers from the *Institute of Theoretical Physics* at RUB
Further information These course components may also be in the RUB Module Handbook for M.Sc. Physics as Module 2b, Advanced Quantum Mechanics