Module	***Theoretical Aspects of NMR Spectroscopy***
Code	
Instruction language	English
ECTS credits	6
Classroom time	5 hours per week
Duration	1 semester
Cycle	Winter semester
Coordinator	Dean of Physics Studies
Lecturers	Dr. Tobias Speidel, Dr. Raiker Witter, Prof. Dr. Volker Rasche
Allocation to study programmes	Physics M.Sc., elective module, 1st or 2nd semester Wirtschaftsphysik M.Sc., elective module, 1st - 3nd semester
Formal prerequisites	None
Recommended prerequisites	None
Learning objectives	Students who successfully passed this module: • understand the fundamentals of spin dynamics and spin/spin interactions in a quantum mechanical picture • understand the fundamentals of nuclear magnetic resonance (spectroscopy) including dedicated applications
Content	• Nuclear spin and its Hamiltonian • Experimental evidence of the (electron and nuclear) Spin • QM treatment of the nuclear Spin (angular momentum operator, single sates and wave function) • Time evolution of a single spin • Introduction of QSM (time evolution of a spin ensemble) • Introduction of spin interactions (multiple spin systems) • Introduction of coherences, relaxation and thermal equilibrium • Excitation and signal detection • Gradient and space encoding (introduction of the k-space, Imaging) • Deduction of the NMR Hamilton operator • Introduction and discussion of NMR interactions (nuclear shielding vs. chemical shift, dipolar coupling, J-coupling, quadrupolar coupling, paramagnetic and knight shift interactions, secular approximations) • Feature of the FT-NMR experiment (pulses, phases, setup, sampling, FFT, S/N) • Density Matrix Description of 2D Experiments (2D-COSY, 2D-HETCOR) • Powder Spectra (chemical shift and quadrupolar coupling) • Spectral resolution enhancement (magic angle spinning, spinning sidebands, chemical shift, dipolar coupling and quadrupolar coupling) • The concept of Echo (rotational echo vs. pulse echo) • Rotor synchronous experiments (pulse sequences)

Literature	• A. Abragam; Principles of Nuclear Magnetism; Clarendon Press; 1983. • C.P. Slichter; Principles of Magnetic Resonance. Springer Series in Solid-State Sciences; Springer Berlin Heidelberg; 1996. • Melinda J. Duer; Introduction to Solid-State NMR Spectroscopy; John Wiley & Sons; 2005. • Atta-ur-Rahman und M. Iqbal Choudhary; Applications of NMR Spectroscopy; Bentham; 2015.
Teaching and learning methods	Lecture with exercise (5 hours per week)
Workload	45 hours lecture (attendance time) 30 hours exercise (attendance time) 105 hours private study Total: 180 hours
Assessment	The module examination consists of a graded written or oral examination, depending on the number of participants. Participation in the examination requires an ungraded study achievement. The type, content and scope of the study achievement will be announced in good time in the course information.
Basis for	Research in the fields of solid state physics, biophysics and medical imaging techniques.