Introduction to Nuclear Magnetic Resonance

Docent: Raiker Witter

Time: 16.10.2023 – 21.02. 2024

25.07.2023

Table of Contents

1 Syllabus

1.1 Basic Considerations

The lecture course is considered to provide the students an introduction into basic theoretical and 46experimental physics concepts of nuclear magnetic resonance,

- **(i)** **introductory:** Stern-Gerlach experiment, Rabi experiment, NMR related noble prices;
- **(ii)** **theoretically:** the spin, wave-function, Schrödinger Equation, Hamiltonian (interactions between electrons and nuclei in context of an external magnetic field – quantum chemical attempts with perturbation theory), Liouville von Neumann Equation, density operator/matrix, time-evolution operator (propagator), equilibrium vs. excited states, multi-quantum coherences, observation/truncation, rotating frame, average Hamiltonian, irreducible tensor formalism, relaxation (fluctuation, autocorrelation, spectral density, transition rates and relaxation times), product operator formalism, etc.; and
- **(iii)** **experimentally:** basic setup (magnetic field incl. gradients, inductive detection, resonance circuit, duplexer, quadrature detection, ADC and computer), signal-to-noise, pulsed experiments, Fourier transformation, spectral fitting, signal assignment, referencing, magic-angle-spinning, rotor-synchronicity, MRI, *ex-situ*, *in-situ*, *operando*, etc.

On the basis of this, an entrance to liquid- and solid-state nuclear magnetic resonance (NMR) will be given by providing application examples in organic, biomedical and inorganic chemistry.

Furthermore, a comprehensive introduction into dynamic nuclear polarization (DNP), electron spin resonance (EPR), quantum-sensing and quantum computing will be provided.

The lecture topics are listed below.

	Week	Topic
1.	16.10.23	Introduction and basic QM Concepts for NMR
2.	23.10.23	NMR-Hamiltonian and Density of Spins
3.	30.10.23	Understanding liquid-state NMR
4.	06.11.23	Examples of liquid-state NMR
5.	13.11.23	Relaxation and Diffusion in liquid-state NMR
6.	20.11.23	Strategies of liquid-state NMR for biomedical Applications
7.	27.11.23	Concepts of solid-state NMR
8.	04.12.23	Experimental Methods in solid-state NMR
9.	18.12.23	Strategies in solid-state NMR for biomedical Applications
10.	08.01.24	Examples of solid-state NMR for inorganic Chemistry
11.	15.01.24	An Introduction to EPR
12.	22.01.24	An Overview of different DNP Approaches
13.	29.01.24	Concepts for NMR/EPR Quantum Sensing
14.	05.02.24	NMR Quantum Computing
15.	12.02.24	NMR Lab-Tour and Examination

1.2 Organisation

Each lecture talk is accompanied by a seminar where solutions of the weekly distributed problem sheets are presented and discussed. This face-to-face contact also provides the opportunity for a Q&A session related the lecture content and beyond.

During the lecture, one day before he examination, a lab-tour will be provided, in order to give the student a practical experience and directly ask questions about the topic.

1.3 Evaluation Criteria

Students are encouraged to solve the problem sheets. In order to become accepted for the lecture's final examination, students have to attempt solving all problems, gain at least 50% of the maximum points and successfully present them at least 3x during the semester's seminars.

Written examinations are considered in the final week during the course time.

A possible re-examinations will be provided during the semester break or first weeks of the follow-up semester.

2 Literature

- Understanding NMR Spectroscopy; James Keeler, Wiley, 2010
- Quantum Mechanics Vol. 1 & 2, C. Cohen-Tannoudji et al., 1977
- Spin Dynamics, M. H. Levitt, 2008
- Principles of Magnetic Resonance, C. P. Slichter, 1978
- Principles of Nuclear Magnetism, A. Abragam, Clarendon Press, 1983
- Introduction to Solid-State NMR Spectroscopy, Melinda J. Duer, John Wiley & Sons, 2005
- Applications of NMR Spectroscopy, Atta-ur-Rahman and M. Iqbal Choudhary, Bentham, 2015
- Electron Paramagnetic Resonance Spectroscopy: Fundamentals, Patrick Bertrand, Springer, 2020
- Handbook of High Field Dynamic Nuclear Polarization, Vladimir K. Michaelis et at., Wiley, 2020
- NMR Quantum Information Processing, Ivan Oliveira et al., Elsevier Science, 2011
- Lectures on General Quantum Correlations and their Applications (Quantum Science and Technology), Felipe Fernandes Fanchini et al., Springer, 2017
- Electron Spin Resonance (ESR) Based Quantum Computing (Biological Magnetic Resonance Book 31), Takeji Takui, Lawrence Berliner et al., 2016