SYLLABUS – CHM6580 Section 11071, Fall 2019

Introduction to Spin Dynamics and Nuclear Magnetic Resonance

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Office Hours: TBA
Class meetings: MWF Period 3 (9:35 AM – 10:25 AM), Flint Hall 0109

OBJECTIVES

The theory and practice of nuclear magnetic resonance (NMR) spectroscopy is introduced. No prior knowledge of the subject is assumed. The theory is developed from the fundamental quantum mechanics of spin, spin interactions, spin dynamics, spin coherence, and spin relaxation. The density operator/matrix formulation of NMR is developed and applied to explain the inner workings of radiofrequency pulse sequences for one and two-dimensional spectroscopy. Levitt's SPINDYNAMICA package (running in Wolfram's Mathematica) is used in tutorials and spectral simulations. Practical aspects of NMR spectroscopy are also be covered, including resonant radio-wave circuits, NMR spectrometer architecture, signal detection, signal processing, and properties of the fast Fourier transform. Three different hands-on laboratory activities are integrated into the curriculum to reinforce the connection between theory and experiment.

PREREQUISITES

An undergraduate level course on quantum mechanics is recommended.

PLACE IN CURRICULUM

This course satisfies the spectroscopy course requirement to qualify for the PhD in the Division of Physical Chemistry.

REQUIRED TEXTS

- Malcolm H. Levitt, Spin Dynamics: Basics of Nuclear Magnetic Resonance (Paperback), Wiley; 2nd edition, ISBN-13: 978-0470511176
- James Keeler, Understanding NMR Spectroscopy (Paperback), Wiley, 2nd edition, ISBN-13: 978-0470746080

REQUIRED SOFTWARE

- Wolfram's Mathematica
- Malcolm Levitt's Spindynamica package (http://www.spindynamica.soton.ac.uk/)

OPTIONAL SOFTWARE

- MestReNova (UF Chemistry site licensed)
- Bruker Topspin (Student edition available, https://store.bruker-biospin.com/shop/US/product/H9966S3/)

SUPPLEMENTAL TEXTS (USED TO PREPARE LECTURES)

- Richard R. Ernst, Geoffrey Bodenhausen, Alexander Wokaun, Principles of Nuclear Magnetic Resonance in One and Two Dimensions (Paperback), Oxford University Press, ISBN-13: 978-0198556473
- B.C. Gerstein and C.R. Dybowski, Transient Techniques in NMR of Solids: An Introduction to Theory and Practice, Academic Press, Inc. (1985) ISBN: 0-12-281180-1.
- M. Duer, Introduction to Solid-State NMR Spectroscopy, Wiley-Blackwell, 1st Edition (2005) 978-1405109147.

GRADING: in-class exams (2 @ 20%), take-home exam (30%), lab writeups (3@10%). Letter grades will be assigned based on the following rubric (subject to change):

>85 %	A	>75 %	B+	>60 %	C+
>80 %	A-	>70 %	B	>55 %	C
		>65 %	B-	>50 %	C-

ATTENDANCE: 100% attendance and class participation are expected.
MAKE-UP EXAMS: Must be arranged in advance of the scheduled date. No make-up exams are allowed otherwise except for emergency situations.
GRADING POLICIES: https://catalog.ufl.edu/ugrad/current/regulations/info/grades.aspx

Week	**Topics**
1.	Two-level systems, spin angular momentum, magnetic dipole moments, spin polarization, vector picture, static and alternating magnetic fields, lab frame Bloch equation, rotating frame Bloch equation, steady-state magnetization, continuous-wave NMR.
2.	Spin quantum numbers, spin states, Dirac notation, Zeeman interaction, introduction to SpinDynamica, Eigenvalue equations, Hermitian operators, unitary operators, powers of operators, exponentials of operators, commutation relationships, raising and lowering operators, trace properties, rotation operators.
3.	Matrix representation of operators, RF pulses, nutation, RF offset effects, ensembles of spins, density operator, populations, coherences, orders of coherence, coherence transfer, thermal equilibrium density operator, Liouville-von Neumann equation, rotating frame density operator, coherence excitation, population inversion, free induction decay, signal calculation.
4.	Phase shifts, receiver reference, linear phase shift, Nyquist sampling theorem, Fourier transform, NMR hardware, spectrometer block diagram, probe circuits, duplexer, receiver, transmitter, digitization, signal processing: left shift, baseline correction, zero-fill, apodization, quad-ghosts, phase correction, peak integration, processing real NMR data.
5.	**LAB #1,** RF lab. Use of the oscilloscope, network analyzer, splitters, mixers, filters, hybrids, directional couplers, attenuators, phase shifts, duplexer, impedance matching and probe circuit tuning.
6.	Coupled spin systems in liquids, quantum states of coupled spins, diagonalization, singlet/triplet basis, Zeeman basis, signals calculation for arbitrary coupling, tensor product, pure states, entangled states. Multi-spin density operator, master equation, product operator formalism part 1.
7.	Product operator formalism part 2: AX_2, AX_3 spin systems, propagators, propagator manipulations, composite pulses, signal calculations, pulse sequences 1: spin echo, J-spectroscopy.
8.	**LAB #2,** Hahn echo, solid-echo, stimulated echo.
9.	Pulse Sequences 2: INEPT (non-refocused), INEPT (refocused), exchange spectroscopy, phase cycling, coherence transfer pathway selection, homospoil, pure absorption 2D spectra, COSY, TOCSY.
10.	**LAB #3,** Collection and processing of 2D NMR Spectra
11.	Spin interactions in solids: chemical shift, dipole-dipole, electric quadrupole, “secular” vs. “non-secular” interactions, solid-state NMR: chemical shift powder patterns, Pake patterns, quadrupolar powder patterns, principle value extraction.
12.	Random field relaxation, fluctuations, spectral density, transition probability, relaxation mechanisms, chemical shift relaxation, homonuclear dipole-dipole relaxation, heteronuclear dipole-dipole, quadrupolar relaxation, relaxation measurements, inversion recovery, CPMG-T2.
13.	NOESY spectroscopy, distance measurements, chemical exchange effects, 1D exchange spectroscopy, 2D exchange spectroscopy, solid-state NMR (magic angle spinning), cross-polarization, dipolar decoupling.
14.	Hyperpolarization techniques: Dynamic Nuclear Polarization and Parahydrogen Induced Polarization.