SYLLABUS – CHM6580, Spring 2022

Introduction to Spin Dynamics and Nuclear Magnetic Resonance

Instructor: Prof. Russ Bowers, Department of Chemistry
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Office Hours: TBA
Class meetings: MWF Period 8 (3:00 – 3:50), Flint Hall 0109
Class dates: 01/05/22-4/20/22

OBJECTIVES

The objective of this course is for students to become competent in the basic theory and practice of nuclear magnetic resonance (NMR) spectroscopy. No prior knowledge of the subject is assumed. State description and matrix representation of quantum mechanics using Dirac (Bra-ket) notation is introduced. The equations describing spin dynamics is developed from the fundamental quantum mechanics of spin and spin interactions. The density operator/matrix formulation of NMR is introduced and applied to explain the inner workings of radiofrequency pulses and sequences of pulses. Levitt's SPINDYNAMICA package (running in Wolfram's Mathematica) is used in tutorials and spectral simulations, and Kuprov's Spinach (running in Matlab) is also employed for 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. Hands-on laboratory activities are integrated into the curriculum to reinforce the connection between theory and experiment.

PREREQUISITES

An undergraduate level understanding of quantum mechanics is recommended. Key principles of quantum mechanics will be reviewed. Spin systems provide an excellent platform for learning quantum mechanics.

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**. Available for free online.**

REQUIRED SOFTWARE

- Wolfram's Mathematica (purchase or access via UFApps)
- Malcolm Levitt's Spindynamica package (free, http://www.spindynamica.soton.ac.uk/)
- Matlab (UF Chemistry site-license available)
- Spinach (free, www.spindynamics.org)
- MestReNova (UF Chemistry site-license)

OPTIONAL SOFTWARE

PDF Scan Software - for scanning your homework pages into PDF for uploading onto Canvas. Genius Scan, by Grizzly Labs, is highly recommended. The app is available for IOS or Android phones. PDF scans cam be directly uploaded to Cloud Storage such as UF Google Drive, Dropbox, or UF OneDrive.
Word Processing - The standard is MS Word with the built-in equation editor. Any other word-processing software with equation editing capability is also acceptable. Fancier equation formatting can be achieved using the MathType plugin from Design Science is optional.
UFApps - UFApps offers a large number of different software packages to UF students free of charge.
UF OneDrive - required for transferring files between your local computer and UFApps.

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.
- Spin Choreography: Basic Steps in High Resolution NMR, Ray Freeman, ISBN-13:978-0198504818.

GRADING: in-class exams (2 @ 20%), final project (15%), lab writeups (3@5%), quizzes (30%). Letter grades will be assigned based on the following rubric (subject to change):

>80 %	A	>74 %	B+	>65 %	C+
>77 %	A-	>71 %	B	>62 %	C
		>68 %	B-	>59 %	C-

ATTENDANCE

If you're going to miss any lecture for any reason, please let the instructor know in advance. Don't be late. I keep tabs on that.

HOMEWORK

Homework will be assigned but not graded. Homework solutions will be provided.

MAKE-UP EXAMS

Must be arranged in advance of the scheduled date. No make-up exams are allowed otherwise except for emergency situations.

Late Submission Policy

Late assignments will receive a late penalty of 10% per day past the scheduled due date. If something arises that prevents you from completing the assignment on time, contact the instructor as soon as possible to request an extension.

GRADING POLICIES: https://catalog.ufl.edu/ugrad/current/regulations/info/grades.aspx

TENATITIVE SCHEDULE

Week **Topic**

1. Spin quantum numbers, spin states, Dirac notation, Zeeman interaction, two-level systems, spin angular momentum, Eigenvalue equations, Hermitian operators, unitary operators, powers of operators, exponentials of operators, commutation relationships, raising and lowering operators, trace properties, rotation operators.
2. 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.
3. 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.

4. Vector picture, static and alternating magnetic fields, lab frame Bloch equation, rotating frame Bloch equation, steady-state magnetization, continuous-wave NMR.
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, principal 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.

UF COVID-19 Statements

1) Our class sessions may be audio-visually recorded for students in the class to refer back and for enrolled students who are unable to attend live. Students who participate with their camera engaged or utilize a profile image are agreeing to have their video or image recorded. If you are unwilling to consent to have your profile or video image recorded, be sure to keep your camera off and do not use a profile image. Likewise, students who un-mute during class and participate verbally are agreeing to have their voices recorded.
If you are not willing to consent to have your voice recorded during class, you will need to keep your mute button activated and communicate exclusively using the "chat" feature, which allows students to type questions and comments live. The chat will not be recorded or shared.

As in all courses, unauthorized recording and unauthorized sharing of recorded materials is prohibited.
2) Lectures and office hours will be conducted through Zoom. The course is managed through Canvas. Course materials will be provided to you with an excused absence, and you will be given a reasonable amount of time to make up work.

More information in the university attendance policies

Getting Help

For the quickest response, you might find it useful to post questions to the Canvas Discussion Board. Messaging the Instructor or even a classmate also works.
For Username/Password issues, such as difficulties logging into any Gatorlink-authenticated site at UF, (including our course website), please contact the UF Help Desk at: helpdesk@ufl.edu, (352) 392-HELP - select option 2.

UF Policies Shaping This Course

This course is aligned with the UF policies below.

- Contact Hours: "Contact Hours" refers to the hours per week in which students are in contact with the instructor, excluding office hours or other voluntary contact. The number of contact hours in this course equals the number of credits the course offers.
- Workload: As a Carnegie I, research-intensive university, UF is required by federal law to assign at least 2 hours of work outside of class for every contact hour. Work done in these hours may include reading/viewing assigned material and doing explicitly assigned individual or group work, as well as reviewing notes from class, synthesizing information in advance of exams or papers, and other self-determined study tasks.
- Accommodation for Student with Disabilities:Students with disabilities who experience learning barriers and would like to request academic accommodations should connect with the disability Resource Center by visiting https://disability.ufl.edu/students/get-started/. This class supports the needs of different learners; it is important for students to share their accommodation letter with their instructor and discuss their access needs as early as possible in the semester.
- Statement Regarding Evaluations:Students are expected to provide professional and respectful feedback on the quality of instruction in this course by completing course evaluations online via GatorEvals. Guidance on how to give feedback in a professional and respectful manner is available from the Gatorevals website. Students will be notified when the evaluation period opens, and can complete evaluations through the email they receive from GatorEvals, in their Canvas course menu under GatorEvals, or viathe evaluation system.Summaries of course evaluation results are available to students at thepublic results website.
- Statement Regarding Course Recording:Our class sessions may be audio visually recorded for students in the class to refer back to and for use of enrolled students who are unable to attend live. Students who participate with their camera engaged or utilize a profile image are agreeing to have their video or image recorded. If you are unwilling to consent to have your profile or video image recorded, keep your camera off and do not use a profile image. Likewise, students who un-mute during class and participate verbally are agreeing to have their voices recorded. If you are unwilling to consent to have your voice recorded during class, you will need to keep your mute button activated and communicate exclusively using the "chat" feature, which allows students to type questions and comments live. The chat will not be recorded or shared. As in all courses, unauthorized recording and unauthorized sharing of recorded materials is prohibited.

University Policy on Academic Misconduct

This class will operate under the policies of the student honor code which can be found at: https://www.dso.ufl.edu/sccr/process/student-conduct-honor-code/. The students, instructor, and TAs are honor-bound to comply with the Honors Pledge: **We, the members of the University of Florida community, pledge to hold ourselves and our peers to the highest standards of honesty and integrity.** You are expected to exhibit behavior consistent with this commitment to the UF academic community, and on all work submitted for credit at the University of Florida, the following pledge is either required or implied: *"On my honor, I have neither given nor received unauthorized aid in doing this assignment*." It is assumed that you will complete all work independently in each course unless the instructor provides explicit permission for you to collaborate on course tasks. Furthermore, as part of your obligation to uphold the Honor Code, you should report any condition that facilitates academic misconduct to appropriate personnel. It is your individual responsibility to know and comply with all university policies and procedures regarding academic integrity and the Student Honor Code. Violations of the Honor Code at the University of Florida will not be tolerated. Violations will be reported to the Dean of Students Office for consideration of disciplinary action. For more information regarding the Student Honor Code, please see: https://www.dso.ufl.edu/sccr/process/student-conduct-honor-code/.

Additional UF Policies and Resources

University Police
The UF police are together for a safe campus. 392-1111 (or 9-1-1 for emergencies) http://www.police.ufl.edu/.
Career Connections Center
Career Connections Center(352-392-1601 |CareerCenterMarketing@ufsa.ufl.edu) connects job seekers with employers and offers guidance to enrich your collegiate experience and prepare you for life after graduation.
Counseling and Wellness Center
Counseling and Wellness Center(352-392-1575) provides counseling and support as well as crisis and wellness services including avariety of workshopsthroughout the semester (e.g., Yappy Hour, Relaxation and Resilience).
Dean of Students Office
Dean of Students Office(352-392-1261) provides a variety of services to students and families, including Field and Fork (UF's food pantry) and New Student and Family programs
Disability Resource Center

- Disability Resource Center(DRCaccessUF@ufsa.ufl.edu| 352-392-8565) helps to provide an accessible learning environment for all by providing support services and facilitating accommodations, which may vary from course to course. Once registered with DRC, students will receive an accommodation letter that must be presented to the instructor when requesting accommodations. Students should follow this procedure as early as possible in the semester.

Multicultural and Diversity Affairs
Multicultural and Diversity Affairs(352-294-7850) celebrates and empowers diverse communities and advocates for an inclusive campus.
Office of Student Veteran Services
Office of Student Veteran Services(352-294-2948 |vacounselor@ufl.edu) assists student military veterans with access to benefits.
ONE.UF
ONE.UF is the home of all the student self-service applications, including access to:

- Advising
- Bursar(352-392-0181)
- Financial Aid (352-392-1275)
- Registrar (352-392-1374)

Official Sources of Rules and Regulations
The official source of rules and regulations for UF students is the Undergraduate Catalog and Graduate Catalog. Quick links to other information have also been provided below.

- Student Handbook
- Student Responsibilities, including academic honesty and student conduct code
- e-Learning Supported Services Policies includes links to relevant policies including Acceptable Use, Privacy, and many more
- Accessibility, including the Electronic Information Technology Accessibility Policy and ADA Compliance
- Student Computing Requirements, including minimum and recommended technology requirements and competencies.

DISCLAIMER

All aspects of course operations, including grading scale, points distribution course policy, and policy execution, are subject to change at the discretion of the course instructor at any time without notice.