SYLLABUS – CHM6580 Section 658B / CHM4930 – Special Topics, Fall 2024

Introduction to Spin Dynamics and Quantum Computing

Instructor: Prof. Russ Bowers, Department of Chemistry
Office: Physics Building 2360
Email: bowers@chem.ufl.edu
Phone: 352 846-0839
Class meetings: T 2-3, R 2, LEI 242
Office Hours: TBA

COURSE DESCRIPTION

Quantum computing uses superposition and entanglement of quantum states to perform computational tasks more efficiently than any classical computer. Systems of coupled spins have played a central role in the development of quantum computing. The first half of the course covers the fundamentals of quantum mechanics of coupled spins and introduces the concepts of superposition, entanglement, pure and mixed states, spin evolution, and decoherence under local and applied interactions. Building on this foundation, the second half of the course focusses on logic gates and their formulation using composite pulses. Finally, examples of quantum algorithms in coupled spin systems will be considered along with experimental demonstrations.

This course is listed as a graduate course as CHM6580 Section 658B and as an undergraduate special topics course as CHM4930.

OBJECTIVES

- Proficiency in the mathematical formulation of quantum states and basic quantum operations in systems of coupled spins.
- Understanding logic gates and their construction using spin qubits.
- Familiarity with initialization and preparation methods.
- Understanding basic quantum computing algorithms.
- Understanding engineering challenges currently faced in the development of quantum computers.

PREREQUISITES

- Linear algebra (recommended but not required). Essential concepts of linear algebra will be reviewed, and an ungraded tutorial will be available to students upon request.

REQUIRED TEXTS

The course will largely follow the two comprehensive review articles by J.A. Jones.

- Jonathan A. Jones, *Controlling NMR spin systems for quantum computation*, Progress in Nuclear Magnetic Resonance Spectroscopy 140-141 (2024) 49–85. https://doi.org/10.1016/j.pnmrs.2024.02.002
- Jonathan A. Jones, *Quantum computing with NMR*, Progress in Nuclear Magnetic Resonance Spectroscopy 59 (2011) 91–120. https://doi.org/10.1016/j.pnmrs.2010.11.001
- L.M.K. Vandersypen, I.L. Chuang, *NMR techniques for quantum control and computation*, Rev. Mod. Phys. 76 (2005) 1037–1069. https://doi.org/10.1103/RevModPhys.76.1037

SUPPLEMENTAL TEXTS AND LITERATURE

The lectures on the fundamentals of spin dynamics and nuclear magnetic resonance will draw on the following sources.

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

The course will also reference the more general texts:

- P. Kaye, R. Lafamme, and M. Mosca, An Introduction to Quantum Computing, Oxford University Press, 2007. ISBN: 9780198570004
- M. A. Nielsen and I. L. Chuang, Quantum Computation and Quantum Information: 10th Anniversary Edition. Cambridge: Cambridge University Press, 2010. ISBN: 9781107002173, https://doi.org/10.1017/CBO9780511976667

SOFTWARE

- Python
- Mathematica (via UFApps)
- Levitt's Spindynamica package (free, http://www.spindynamica.soton.ac.uk/)
- Matlab (UF Chemistry site-license available)

GRADING

Homework	10%
Midterm	30%
Final Exam	30%
Term Project	30%

ATTENDANCE

If you're going to miss any lecture, please let the instructor know in advance. Please be punctual. **More information in the university attendance policies.**

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 on Homework and Reports

Late assignments will receive a late penalty of 25% per day past the scheduled due date.

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

TENATITIVE SCHEDULE

Week	Topic
1.	Spin states, Dirac notation, Schrodinger equation, spin operators, operator identities, rotation operators.
2.	Matrix representation, diagonalization, RF fields, Rabi nutation.
3.	Ensembles of spins, density operator, populations, coherences Liouville-von Neumann equation.
4.	Rotating frame density operator, free evolution, LVN equation, NMR observables.
5.	Nyquist sampling theorem, Fourier transform, signal processing.
6.	Systems of coupled qubits, singlet/triplet basis, Zeeman basis, tensor product.
7.	Orders of coherence, pure states, superpositions and entangled states.
8.	Product operator formalism
9.	Transition selective pulses, composite pulses, qubit readout.
10.	Molecular spin systems, DiVencenzo criteria.
11.	Logic gates: global phases and logic gates, single qubit gates, controlled gates.
12.	Preparation and initialization methods, pseudo-pure states, hyperpolarization.
13.	Algorithms 1. Deutsch's algorithms.
14.	Algorithms 2. Grover and search algorithms,
15.	Algorithms 3. Shor type algorithms, adiabatic algorithms.

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 via the evaluation system. Summaries of course evaluation results are available to students at the public 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.