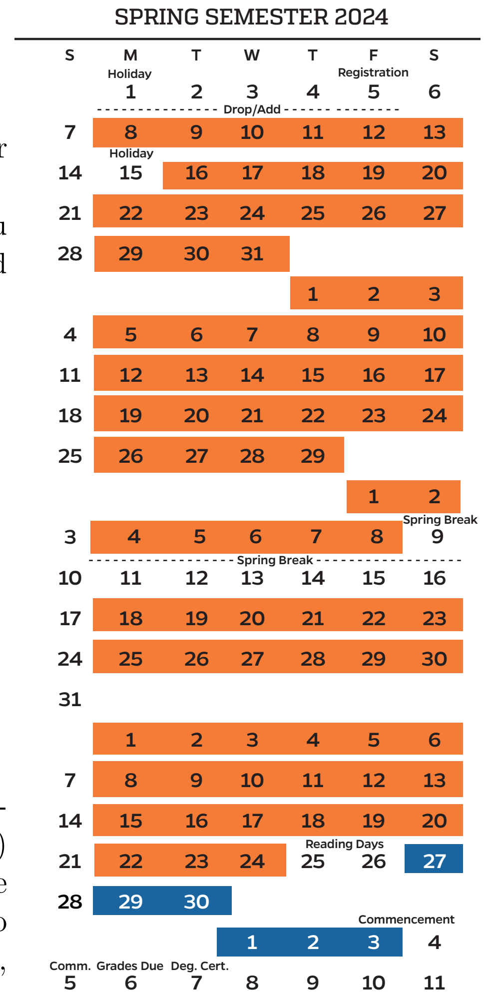
CHM4412:
Quantum Mechanics and Spectroscopy

Spring 2024 4 credit hours

Class Number(section): 10800 (PF12)

T R Periods 4 - 5 (10:40 - 12:35) LEI207



No (specifically) Required Textbook:
Useful texts include *the one you have* or something like:
Physical Chemistry, P. W. Atkins *et. al.*, any addition, or similar titles by McQuarrie & Simon, Levine, Raff, Castellan
Complete notes for this course will be provided online. However, you also *need* a textbook, in addition to these notes, as multiple sources and perspectives will augment your breadth of understanding.

Contact Brucat if you have questions...

Instructor: PJ Brucat

- Office hours (subject to optimization):
  TBA
  TBA
  or by appointment (message three choices)
- Contact method: *Canvas Messaging only* (No email)

TA: Alexander Kim

Course Website:
https://ufl.instructure.com/courses/497232
All communication and activities related to this course will be accessible from within UFs campus-wide eLearning system (Canvas) at the URL above. Please become familiar with our course website as soon as possible. Much of the materials there are be subject to revision, so pay careful attention to all announcements, updates, and revision dates. *It is strongly advised that hardcopy or static downloads of course materials be avoided due to their continuous incremental improvement.*

Etiquette

Your polite, courteous, and civilized behavior is expected in all aspects of our course. This holds especially true in these times of stress and uncertainty. Be Human.

Recordings

State law permits unregulated, unannounced audio and/or video recording of all aspects of course meetings without prior consent 'for personal use', whatever that means. Therefore, all participants should assume that they are being recorded at all times.

Goals and Objectives

Course Goals

Successful completion of this course will enable the student to:

- Integrate the Scientific Method into the Investigation of the Natural World
- Apply the Postulates and Methods of Quantum Mechanics to Chemical Problems
- Interpret the Mathematical Description of Microscopic/Molecular Systems
- Employ Fundamental Properties of Chemical Bonds and Bonding to Describe Matter
- Incorporate the Mathematics of Symmetry into the Description of Chemical Behavior
- Formulate Spectroscopic Experiments to Investigate Atoms and Molecules
- Program Computational Tools for Symbolic and Numerical Solutions to Chemical Problems

Course Objectives

Accomplishment in the course material will be assessed in the following:

Knowledge

- Guiding Principles of Mechanics
- Operators, Wave Functions, and the Schrödinger's Equation
- Eigenstates, Uncertainty, and the Act of Measurement
- Time Dependence and Superposition of Quantal Systems
- Representations and Operator Algebra
- Approximate Methods in Quantum Mechanics
- Properties of Simple Systems (PiB, SHO, Rigid Rotor, H Atom, H_2 Molecule, *etc.*)
- Classification and Consequences of Molecular Symmetry
- The Hierarchical and Quasi-Separable Nature of Molecular Motion
- Models of Chemical Bonding
- Semiclassical Interaction of Light with Matter
- Fundamentals of Common Spectroscopic Methods (UV-Vis, IR/Raman, $\mu\lambda$, NMR, *etc.*)
- Non-Linear and Coherent Methods in Modern Spectroscopy

Skills

- Use of Computational Tools in the Solution of Complex Chemical Problems
- Synthesis of a Quantum Mechanical Equation of Motion for an Arbitrary Atomic or Molecular System
- Application of Differential Equation Methods to the Solution of Quantum Mechanical Problems
- Application of Linear and Operator Algebra to the Solution of Quantum Chemical Problems
- Selection and Application of Appropriate Approximate Methods to Quantum Mechanical Problems
- Application of Group Theoretical Methods to Simplify Quantum Mechanical Problems
- Analysis and Interpretation of Molecular Spectra for the Purpose of Extracting Chemical Information

Course Operation

Course Meetings

There are several meeting types intrinsic to the learning experience of this course.

1. **Scheduled Class Meetings** This course has regularly-scheduled meeting times designated for synchronous meetings of the entire class. These meetings are a one-on-many environment primarily for discussion and explanation of new material outlined in the course Attendance in these meetings is *strongly encouraged* but not required. However, your Classroom Participation grade will severely suffer if you are not present in our synchronous discussions. See below for further clarification.
2. **Scheduled Office Hours** The purpose of regularly-scheduled 'office hours' is primarily to assist students as individually as possible in their specific learning needs. It is sometimes a one-on-one activity, but often the collective questions of a a few like-minded students can be even more profitable. These activities are optional, but recommended if a learner finds themselves 'stuck' or frustrated in their advancement. Assistance and 'hints' towards the completion of the classwork and quizzes is also available here. See the Canvas Calendar for the schedule.
3. ***Ad Hoc* Conferences** Any student may request an *ad hoc* one-on-one meeting with the instructor, for whatever purpose, at any time. Such requests will be made exclusively through Canvas Messaging. Requests must include three distinct times for the requested meeting in the initial message and whether the meeting is desired to be private or open to other students, face-to-face or virtual. The Instructor will respond to the request within 12 hours (usually much less) by accepting one of the times and provide a video conferencing link or physical location for the meeting. Such conferences are not restricted to normal business hours, but may be constrained by conflicts with other meetings, health concerns, and mundane extraneous commitments.

Communication with your Instructor

To guarantee rapid, reliable, and secure transmission, all course communications with your instructor(s) are to occur within the Canvas environment using the embedded tools. Configure your Canvas account profile for immediate automatic notification of course announcements and updates, and make sure that email forwarding, if desired, is set up correctly. It is expected that all replies to messages between instructor and student occur within 24 hours. Responsibility for receiving and responding to electronic course communication in a timely fashion is entirely that of the student.

Course Activities

Synchronous Discussion

Twice a week, the entire class will meet for two hours to discuss Quantum Mechanics, its experimental verification (Spectroscopy) and application of both these ideas to Chemical Problems. These meetings are the core of the course, at least as far as the traditional definition of the University curriculum goes. To optimize your time and learning, these class discussions should involve active participation, which, in turn, requires individual preparation and review. To emphasize the necessity and importance of the interactivity expected in these meetings, a Classroom Participation score, determined by the instructor, will be part of your Course Grade computation.

- Preparation For a discussion among a learning community to be profitable, preparation and a common reference must exist. Before every class meeting, the material to be covered that session (see Meeting Schedule) will be reviewed by careful reading of the course notes as well as aggregation of any additional material needed by the individual learner. It is highly recommended that each student keep a detailed notebook which should include documentation and details of the learning process. Any questions or comments that arise in the preparation period should be recorded in the notebook and brought to the class meeting.
- Classroom Participation Our synchronous discussions will begin with a socratic review of the important points of previous topics. This will consist of the instructor asking students about those topics, and a discussing them. Throughout the meeting, questions from students regarding material of the day are encouraged. At the conclusion of the meeting, concept questions, sometimes closely related to the Concept Quizzes will be posed to summarize the topics of the day. A subjective grade associated with individual student participation will be assessed by the instructor..

Office Hours

Every student of Physical Chemistry is unique. The classwide discussions of the topics are necessarily a compromise, in that your instructor must target the group collectively, and thus imperfectly. It is expected *and encouraged* that each student take advantage of individual meetings with the instructor.

Formative Assessments

Physical Chemistry is a journey; Mastery of it is the goal. We will progress towards mastery through activities that challenge us and help us focus and apply our learning. There will be two types of these activities, subsequently called *assignments*:

Concept Quizzes (CQ) Periodically throughout the term, short question sets will be delivered online through our course website. These are intended to be *formative* assessments, in that these activities focus on and cement concepts in the learners mind. These quizzes are entirely based on material in the course notes and are to be worked individually. That means you may only discuss the quiz and its contents with your instructor until after the due date.

Course Work (CW) Class Work is a set of exemplary problems to challenge your skill and cement your mastery of the material. These are approached by the individual student asynchronously. Collaboration is allowed and encouraged. However, each student must submit their own individual work for grading by the instructor. Submitting someone else's work not only impedes the instructors ability to assist your learning but is also a violation of the Honor Code.

Meeting Schedule

(tentative; see Canvas website course stream)

Week	Date	Lec	Topic	Notes Chapter
1	01/09	01	Syllabus, Operation, and Introduction to Mechanics	0-1.3
	01/11	02	Virial Theorem; Classical Oscillation; Operators	1.4-2.6
2	01/16	03	Wavefunctions; Uncertainty; Dirac Notation	2.7-3.7
	01/18	04	Completeness; Commutation Relations; Free Particle	3.8-4.1
3	01/23	05	Confinement: The 1-D Particle in a Box	4.2-4.3
	01/25	06	Superposition and Time Dependence	5.1-5.4
4	01/30	07	The Quantum Mechanical 1-D Simple Harmonic Oscillator	6.1-6.4
	02/01	08	Dimensions and Degeneracy	7.1-7.3
5	02/06	09	Creation and Anhilation Operators; the SHO revisted	8.1-8.3
	02/08	10	Approximate Methods in Quantum Mechanics	9.1-9.2
6	02/13	11	The 1-electron Atom; Bohr Model; QM Spherical Solutions	10.1-10.5
	02/15	12	Rigid Rotation; Spherical Harmonics; H Atom eigenstates	10.6-10.7
7	02/20	13	Electron Spin; Atomic Aufbau	11.1-11.4
	02/22	14	Angular Momentum Addition; Atomic Terms; Hund's Rules	11.5-11.6
8	02/27	15	The Chemical Bond; The H_2^+ Ion	12.1-12.5
	03/29	16	Diatomics; MO and VB wavefunctions; Polyatomics	12.6-12.10
9	03/05	17	Molecular Symmetry	13.1-13.6
	03/07	18	The Symmetry Bowl (Identification of Point Groups)	—
10	–	–	— Spring Break —	—
11	03/19	19	The Theory of Simple Groups	14.1-14.7
	03/21	20	Symmetry and Quantum Mechanics	15.1-15.7
12	03/24	21	The Boltzmann Distribution; The Partition Function	16.1-16.5
	03/28	22	Thermo Properties ; Allosterism	16.6-16.8
13	04/02	23	Molecular Dynamics	17.1-17.4
	04/04	24	Blackbody Radiation, Radiometry	18.1-18.5
14	04/09	24	Absorption and Emmision of Light; Resonance; Lineshapes	18.5-19.9
	04/11	25	Photophysics; LIF; Ro-Vibrational Spectra	20.1-20.7
15	04/16	26	Spin and Spin Ensembles	21.1-21.3
	04/18	27	Anisotropic Relaxation	20.4
16	04/23	28	Coherence, Relaxation and NMR Spectroscopy	20.5-20.7
	04/25	–	Reading Day	—

Notes Document: Part 1 ; Part 2 ; Part 3 ; Part 4 ; Part 5

Assignment Schedule

(tentative; see Canvas website course stream)

Week	Assignment	Due Date	Assignment	Due Date
1	CQ00	01/10	CQ01	01/12
2	CW01	01/17	CQ02	01/19
3	CW02	01/24	CQ03	01/26
4	CW03	01/31	CQ04	02/02
5	CW04	02/07	CQ05	02/09
6	CW05	02/14	CQ06	02/16
7	CW06	02/21	CQ07	02/23
8	CW07	02/28	CQ08	03/01
9	CW08	03/06		
10				
11			CQ09	03/22
12	CW09	03/27	CQ10	03/29
13	CW10	04/03	CQ11	04/05
14	CW11	04/10	CQ12	04/12
15	CW12	04/17	CQ13	04/19
16	CW13	04/24		

All 'official' activity dates and grades are posted on the secure course website. Assignments are to be submitted in full by the assignment deadline for credit.

Course Resources and Ancillary Materials

- **Content**
  - **Textbook**
    This course covers material that is part of the core of any Physical Chemistry curriculum. Therefore, it is covered in many ways in many published, professionally edited and proofread textbooks. New Physical Chemistry textbooks are expensive, but recent but not current, editions can be acquired for little money and remarkable value. Get some. Use the Marston Library, https://marston.uflib.ufl.edu/ to peruse a large variety of text resources related to our course.
  - **Course Notes**
    Notes guiding course topics and discussion are posted on the course website. The expectation is that these notes guide your preparation prior to attending the class meetings. It is not expected that these notes will be sufficient on their own for all learners to master the subject matter, but this is the ultimate goal. As a draft document, these notes will be revised constantly through the term; Please always refer to the latest revision date.
- **Mathematics Tools**
  Mathematics is the language of Physical Chemistry. However, Math skills should not be a stumbling block for learning Quantum Mechanics and Spectroscopy. There are many modern tools that can assist *anyone* in the execution of mathematical procedures and manipulations that it would have taken a genius to perform a few generations ago. Can't take a derivative or perform an integral? There are tools for that. Need to perform tedious iterative approximations? There are tools for that too. There are tools for virtually every aspect of every calculation in this course. Make use of them.

··· **Python/Jupyter**
Right now, the most popular scientific computing 'language' is Python. It is ubiquitous in Chemistry and has lots of community support. There are libraries (packages) for almost everything a Chemist wants to do already written in Python, so it is an obvious choice for a student without other expertise. For anything other than routine computation, most scientists use Python in an interactive UX as delivered in Jupyter through a cell-based 'notebook'. This environment resembles some of the features of the *Mathematica* app, but has two advantages: It is community-supported an open source (free!), and it is becoming a standard for use by Chemical researchers, data scientists, and many other smart people. This means familiarity with Python in some form may just be what it takes to get you a job. At the very least it will be useful for whatever career path you follow. So, how does one get started with Python notebooks? Some choices:

1. *Install "Anaconda" on your own device* (Recommended regardless of other options) 'Anaconda' is a code suite that allows one to easily setup Jupyter/iPython/R on your own device. If you are in possession of a laptop or desktop and do any sorts of analysis with it, you should have Anaconda installed. The free download and instructions can be found on the website: https://www.anaconda.com/distribution/. Anaconda is also available through UF apps, in case you want a test drive.
2. *Use the Chemistry Jupyter Server* (Recommended for graded assignments in this course) A ready-to-go, web-accessible, Jupyter server has been created for use in this course. If you put your work their, the instructor can look at it immediately when questions arise and provide tips and hints right in your notebook. The server can be found here: https://jupyter.chem.ufl.edu:8000/. Login there with your Gatorlink username (the part of your @ufl.edu email address before the @ symbol) and the initial password "mechanicup". Instructions for changing your password to protect your work will be provided on the curse website. Note: If off campus, VPN into the UF network before hitting the login page.
3. *Google Colaboratory* (Access GPU and TPU capability) The fine people at Google have provided a full-featured Jupyter server for public use near https://colab.research.google.com/. There are a few limitations to this service, but it is a way to execute an *.ipynb notebook on your Google Drive. Execution with advanced hardware options and with non-standard packages is possible with a bit of expertise. This service is invaluable in a pinch, or if you have to run a quick calculation or plot when away from your normal resources.

··· **Quantum-Chemical-Specific Calculation Tools (WebMO)**
There are several sophisticated software packages available for the computation of the electronic structure of isolated molecules. These tools are extremely useful in testing and learning the concepts of Quantum Mechanics in their application to Chemistry. A few of the most powerful tools have been aggregated and access provided to you through a web interface called "WebMO". The login for students of this course is here: http://webmo.chem.ufl.edu/~webmo/cgi-bin/webmo/login.cgi Login with your Gatorlink username (the part of your @ufl.edu email address before the @ symbol) with the initial password "mechanicup" (without the quotes). Change your password immediately ("Utilities" ⇒ "Edit Profile") to protect your work. Do not use your 'real' Gatorlink password. If off campus, VPN into the UF network first. The use of this tool will be discussed at the appropriate time in the semester, but feel free to wade around at any time.

··· **UF Apps** (Useful if all else fails)
UF students have a powerful suite of software tools available to them via the UF Apps web

(Citrix) interface. Included in these "apps" are some quite sophisticated tools to assist in the symbolic and numerical solution to mathematical problems as well as the visualization of these results. A few that should be familiar are *Mathematica* (The best IMHO), Maple, MatLAB, R, SAS, SPSS, among others. Some of these packages are great, but quite expensive outside of the access provided by UF (*Mathematica*!). UF apps does not provide an alternative to the features provided through WebMO, unfortunately.

··· **HiperGator 3.0** (For heavy lifting)
UF has one of the fastest (and greenest) supercomputers in an academic environment. If you are performing undergraduate research, access to this fantastic resource through that participation is probably already available. If not, and you have any reason (really, *any* reason) to use HiPerGator in the context of this course, temporary access can be requested. It would be thrilling to do this, so think hard about what you might want to learn and go for it.

Teaching and Learning Context

A little over a 100 years ago, no human actually fundamentally understood the nature of matter, or light, or how they interact. Yet, up to that point in history, humans were really pretty good at *manipulating* light and matter. Chemistry, too, as a methodology was fairly well established and powerful. The brute force of the scientific method, fueled by the insatiable need to control and manipulate the environment in which we live, allowed humans to *engineer* capable technologies. But, coherent [*sic*] and complete understanding of the microscopic driving forces of nature were largely mysterious.

At the turn of the 20^{th} century, human ignorance was confronted with a series of inexplicable observations, which forced the acceptance of strange and uncomfortable ideas, a subset of which is called Quantum Theory. These ideas lead to an explosive growth in Science, and most importantly Chemistry, with all its related technologies, enjoying fantastic new capabilities. The predictions of this Quantum Theory are testable, and have thus far proven to be robust. However, the quantum world is so alien and bizarre that its *interpretation* is still in debate among very smart people to this day.

To a certain extent 'interpretation' is a problem in Philosophy, not Chemistry, and therefore somewhat moot. The predictions of a theory can be tested and verified; the 'why' not so much. However, to a student of Quantum Mechanics, such interpretation(s) <u>are</u> important, if not crucial, to the learning process. But, unlike many other areas of study, these interpretations have a tendency to *change* as understanding matures. What is immutable, however, is the *process* by which the development of Quantum Mechanics, or any theory is approached: Make some assumptions, Employ irrefutable logic (Mathematics) to those assumptions to make predictions, and test those predictions with experiment. If all goes well, a discord is found between the predictions and the truth, and something is learned, *i.e.* new and better assumptions are needed. If the boring agreement between predictions and observation results, Bolder predictions are made until something breaks. This is the Scientific Method: Learning by Breaking Things.

Experiments will not be performed first hand in this class, but experimental results from human history (and your associated laboratory courses) will be brought to bear. We will explore the path from assumptions to predictions in much the same way the ancients did (but with fewer missteps) and try to develop interpretations of these predictions that we *as individuals* believe. Your interpretation of Quantum Mechanics may be different than mine, which is perfectly fine, as long as accurate predictions are made from our respective philosophies. The important thing to remember is one has to develop *their own* interpretation of the microscopic world which cannot be gifted or copied (sadly).

For each student to be able to make their own interpretation of Quantum behavior, the path between assumption and prediction must be understood. That means Math. Some of this Math may not be familiar to you, and some of it is just plain cumbersome. Unlike the ancients, we have tools to help us with the Math that will lead us to enlightenment without needless toil. These tools will be integrated [*sic*] into our discussions and are valuable not just for this study, but for problem solving and data analysis of all types. You may find that the exercises in symbolic and numerical computation explored in this course are some of the most valuable and long-lasting benefits of your efforts.

Grades

Course Grade Computation

Research has shown that assessing grades through a few, high-stakes, proctored activities (aka 'Exams') is not the best way to foster deep learning or long-term retention of concepts. Therefore, this course will attempt to have no mid-term or final exams. Course grades will be computed from the weighted-average of the earned percentages of each graded items described in section Course Activities, submitted by the individual student. The weighting factors of the activity categories are as follows:

Default Category Weights

Grade Category	weight %
Class Participation (CP)	25
Concept Quiz (CQ)	25
CourseWork (CW)	50

Alternate Category Weights

Grade Category	weight %
Class Participation (CP)	15
Concept Quiz (CQ)	10
CourseWork (CW)	25
Final Exam	**50**

If either the instructor or the student body indicate their dissatisfaction in the accuracy of the default grading method, or there is any indication of improper or dishonest behavior in the execution of the assignments, an alternate, more plebeian, grading procedure will be activated. This scheme emphasizes a proctored, cumulative, extremely high-stakes Final Exam. This Final Exam, if necessary, is scheduled as per the OUR. If it is to occur, the activation of the alternate grading scheme for the course will be announced at least two weeks before that date.

The grading scheme will generate an aggregate assignment percentage, which will be converted into a letter grade as follows:

Course Letter Grade Percentages

Grade	A	A−	B+	B	B−	C+	C	D	E
Minimum percentage	87.5	80.0	77.5	72.5	70.0	67.5	60.0	50.0	< 50.0

Regrade Requests

Grade accuracy is a high priority for this course. Assignments will be regraded if a grading error is suspected. Regrade requests from students must be submitted through Canvas Messaging to Brucat within 48 hours of the grade post. Regrades will be performed on the entire assignment following the standard assignment rubric. Grade adjustments may be positive or negative.

UF's Grading Policy

See https://catalog.ufl.edu/UGRD/academic-regulations/grades-grading-policies/

Honesty and Truthfulness

Ethical, moral, and professional behavior is expected and required of all participants in this course. Moreover, all participants in UF's Academic activities are bound by Rules of Conduct, from which can be found the following excerpt:
"UF students are bound by The Honor Pledge which states,
'We, the members of the University of Florida community, pledge to hold ourselves and our peers to the highest standards of honor and integrity by abiding by the Honor Code.'
On all work submitted for credit by students 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'
The Honor Code (http://www.dso.ufl.edu/sccr/process/student-conduct-honor-code/) specifies a number of behaviors that are in violation of this code and the possible sanctions. Furthermore, you are obligated to report any condition that facilitates academic misconduct to appropriate personnel. If you have any questions or concerns, please consult with the instructor or TAs in this class"

Additional Information

Accommodations

The Disability Resource Center at UF offers this advice:

"Students with disabilities who experience learning barriers and would like to request academic accommodations should connect with the Disability Resource Center by visiting our Get Started page. 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."

Counseling

Useful non-academic services are available in many forms at UF.

- U Matter, We Care: If you or a friend is in distress, please contact umatter@ufl.edu or 352 392-1575 so that a team member can reach out to the student.
- The Counseling and Wellness Center: http://www.counseling.ufl.edu/cwc/

GatorEvals

The UF course evaluation policy includes the following statement:

"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 at https://gatorevals.aa.ufl.edu/students/. 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 https://ufl.bluera.com/ufl/. Summaries of course evaluation results are available to students at https://gatorevals.aa.ufl.edu/public-results/."

All course policies and procedures are subject to change at any time at the sole discretion of Brucat

We, the members of the University of Florida Community, pledge to hold ourselves and our peers to the highest standards of honesty and integrity

— Revision: December 25, 2023—