1 LOCATOR INFORMATION

Lecture schedule: MWF 11:00-11:50 AM, LS 304 W

Lecturer: Dr. Jairo Castillo-Chará

Office: S and T 313

Telephone: (910) 672-2062

Office Hours: M 8:00-9:00AM, TR 9:00-11:00AM, MWF 10:00-11:00AM and by appointment

e-mail: jcastill@uncfsu.edu

Website: http://faculty.uncfsu.edu/jcastill/

FSU Policy on Electronic Mail: Fayetteville State University provides to each student, free of charge, an electronic mail account (username@uncfsu.edu) that is easily accessible via the Internet. The university has established FSU email as the primary mode of correspondence between university officials and enrolled students. Inquiries and requests from students pertaining to academic records, grades, bills, financial aid, and other matters of a confidential nature must be submitted via FSU email. Inquiries or requests from personal email accounts are not assured a response. The university maintains open-use computer laboratories throughout the campus that can be used to access electronic mail.

Rules and regulations governing the use of FSU email may be found at http://www.uncfsu.edu/PDFs/EmailPolicyFinal.pdf
2 COURSE DESCRIPTION

This course is an attempt to present the essential ideas of quantum mechanics hopefully in a way that would be interesting, comprehensible and enjoyable to the students with a background of one year of college calculus and physics. The lectures in this class will cover non-relativistic wave mechanics, molecular spectroscopy and introduction to statistical thermodynamics.

2.1 MOTIVATION

You may ask yourself why do you should study quantum mechanics? The answer is that our industrial and technological worlds have evolved at to the point that the new promising developments will be in the nano and atomic size scales. Therefore we should learn to use quantum mechanics in order to be able to describe, understand and control things in the atomic world. For the chemists working in synthesis of organic or inorganic compounds quantum mechanics provide the means to understand mechanisms and dynamics processes through which reactions occur, biologists working with DNA can track the processes\(^1\) in a given atom or group of this huge molecule by attaching a fluorophore to the group or atom that they want to study, then the fluorescence of the attached group can provide details of the dynamics in one section of the molecule. In the area of electronics and material science is worth to mention that a considerable number of new opto-electronic devices, semiconductor transistors and lasers will operate based on the laws of quantum mechanics. As new technology is being developed in these areas, the new devices will considerable shrink in size to the point that it is predicted that for the year to 2030 the cell size of random access memory devices will be less than the size of an atom.\(^2\) This implies that a radical change in the science curriculum need to take place in order to prepare science students with a background in quantum mechanics that will allow them to compete in the job market and to be able to contribute in the new developments of the science and technology of the future. This course is just a first attempt to provide the science students with a considerable background in the fundamental principles of quantum mechanics and some of its applications.

2.2 Prerequisites

This course assumes that the students have taken one year college calculus and physics. An introduction course to differential equations and linear algebra will be useful, however provisions will be

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\(^1\)S. Weiss, Science 283,1676 (1999)

make during the course to satisfy this requirements.

3  DISABLED STUDENT SERVICES:

In accordance with Section 504 of the 1973 Rehabilitation Act and the Americans with Disabilities Act (ACA) of 1990, if you have a disability or think you have a disability to please contact the Center for Personal Development in the Spaulding Building, Room 155 (1st Floor); 910-672-1203.

4  TEXTBOOK


5  STUDENT LEARNING OUTCOMES:

The course will allow students to learn the basic ideas of quantum mechanics as applied to chemistry, to develop critical skills for using mathematical models, theories and to understand their limitations and range of applicability, to develop critical thinking skills that will allow to understand how chemistry operates at microscopic level, and to develop logical thinking patterns that will allow students to understand physical models in mathematical form. More specific with the completion of this course students will be able to understand and learn:

1. the experiments that illustrate the failures of classical physics.
2. the postulates of quantum mechanics and their implications in chemistry.
3. The Schrödinger wave equation and its solution for physical systems relevant to chemistry.
4. The quantum mechanics of translational, vibrational and rotational motion.
5. The atomic, molecular orbitals, probability distributions and their relevance to atomic, molecular structure and chemical bonding.
6. The molecular basis of thermodynamics.
7. The fundamentals to be prepared to take advanced, senior-level and graduate courses in chemistry, biochemistry and physics.
6 COURSE REQUIREMENTS AND EVALUATION CRITERIA:

6.1 HOMEWORK POLICY

To facilitate learning and to be able to accomplish the outcomes outlined above two types of homework will be given:

Basic Concepts Homework (BCHW): Simple conceptual questions about each chapter will be given to get students trained in the fundamentals. Please, look this assignment on the homework assignment section of this document

Problem Solving Homework (PSHW): In this homework students will be able to apply the basic concepts mentioned above and also to practice the different types of problem solving methods discussed in the lectures. This assignment will be posted in blackboard.

1. Homework will be given during Friday class once every week and should be submitted on the following Friday before the start of the class.
2. Homework problems should be neatly written in order to make clear that the instructor understands your solutions (not credit will be given for confusing, unreadable work)
3. Each time that you submit the homework make sure that you write your name, date and problem set number or chapter.
4. Homework submitted late will be graded at a rate of 10 % per day late (you will lost 10 points per day late)
5. Questions about homework or questions related to grading will be discussed during office hours. If you can not see the instructor at the office hours cited above, you can email or call to make an appointment that suit your schedule.
6. The final due date for any assignment (homework, exams and projects) is by 5:00 PM of the day of the final exam date. After this date no assignments will be accepted.

6.2 GRADES

This course will be graded on a maximum of 100 points distributed as follows:

Your course grade will be determined using the total number of points that you have accumulated during the semester.
### Section Points

<table>
<thead>
<tr>
<th>Section</th>
<th>Points</th>
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<tbody>
<tr>
<td>Three hour Exams</td>
<td>45 Points</td>
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<tr>
<td>Final Exam</td>
<td>25 Points</td>
</tr>
<tr>
<td>Homework</td>
<td>30 Points</td>
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<tr>
<td><strong>Total</strong></td>
<td><strong>100 Points</strong></td>
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### Percentile Points Letter Grade

<table>
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<tr>
<th>Percentile Points</th>
<th>Letter Grade</th>
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<tbody>
<tr>
<td>92 - 100%</td>
<td>A</td>
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<tr>
<td>83 - 91%</td>
<td>B</td>
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<tr>
<td>73 - 82%</td>
<td>C</td>
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<tr>
<td>64 - 72%</td>
<td>D</td>
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<tr>
<td>63 or less %</td>
<td>F</td>
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</tbody>
</table>

## 6.3 REVISION OF GRADES STUDENTS RESPONSIBILITIES

Absences from class will be handled following strictly the University policy. Absences of more than 10% of the total contact hours the course meets during the semester, which is approximately seven (7) total hours of unexcused absences will fall in the category of ‘EXCESSIVE ABSENCES-EA’. As indicated in the new guidelines, ‘WN’ grade has been eliminated and it is the STUDENT’S RESPONSIBILITY TO WITHDRAW HIMSELF OR HERSELF FROM THE CLASS. Please, check the 'Revision of Grades-Student Responsibilities’ at: www.uncfsu.edu/fsuretension/policiesprocedures.htm.

- **X GRADE (NO SHOW):** will be assigned to any student on the roster that did not attend during the first week of classes or, in online classes, did not interact with class website during the first week of classes. Since X grade is not a final grade, it can removed if the student begins attending class.

- **EA GRADE (EXCESSIVE ABSENCES):** will be assigned to students whose absences exceed 10% of class contact hours. After the grade has been assigned the student will be warranted in order for them to take the corrective action.

**NEW FINAL GRADE:**

- **FN (FAILURE DUE TO NON-ATTENDANCE):** Final grade for students who are on class roster, but never attend the class. An FN grades is equivalent to an F grade in the calculation of the GPA.
7 STUDENT BEHAVIORAL EXPECTATIONS

1. Students are expected to arrive to class on time, remain in class until dismissed by the instructor, and refrain from preparing to leave class until it is dismissed.
2. Students should avoid passing notes or carrying on private conversations while class is being conducted.
3. Students should avoid the use profanity in the classroom.
4. Any form of cheating is considered an academic dishonesty or misconduct and will be punished. For information about disciplinary measures and university policies for academic misconduct, read the Fayetteville State University Student Handbook.
5. Students should avoid the use of cell phones during exams and class time, this affects the concentration and distract your peers.
6. The use of programmable calculators is strictly forbidden during exams and quizzes, try to bring a simple no programmable calculator if you need one during the exam. Avoid the use of cell phones during the exam and class time, this affects the concentration and distract your peers.
7. The inappropriate use of texting, making calls, taking pictures, etc with cell phones during tests and quizzes is absolutely forbidden and will be punished accordingly if cheating is suspected and proof.

8 CONSEQUENCES FOR FAILING TO MEET BEHAVIORAL EXPECTATIONS

With first time violation of one of the rules above, he or she will be warn privately by the instructor after or before next class. Second time violations will be punished by deducting as many as twenty points from the student’s next exam grade. With third time violations, the student will be reported to the Dean of Students for disciplinary action according to the FSU Code of Student Conduct.[8]

9 ACADEMIC SUPPORT RESOURCES

The instructor will try to make available any additional material such as hand outs and homework that will be required for the proper instruction of students through blackboard (http://blackboard.uncfsu.edu) and the instructor web site (http://faculty.uncfsu.edu/jcastill/).
10 COURSE OUTLINE

I. Introduction to Quantum Theory  
A. Historical perspective  
B. Failure of classical mechanics  
1. Blackbody radiation  
2. The photoelectric effect  
3. The Compton scattering  
4. Wave properties of particles  
5. The Bohr model  
C. The development of quantum theory  
1. The Schrödinger equation  
2. The Born Interpretation of the wavefunction  
3. Mathematical behavior of the wavefunction  
4. The Heisenberg Uncertainty Principle  
5. Operators and observables  
6. Expectation values  
7. Superposition of states  
8. The postulates of quantum mechanics

II. Application of Quantum Theory  
A. The free particle - translational motion  
B. The particle in a box  
C. Barrier penetration  
D. The harmonic oscillator - vibrational motion  
E. Motion of a particle on a circle - rotation in a plane  
1. Quantum Theory treatment  
2. The angular momentum operator \( L_z \)  
F. Rotation on a sphere  
1. Orbital angular momentum  
2. Spin angular momentum

Exam#1 Feb. 3rd week

III. Atomic Structure and Spectra  
A. Hydrogenic atoms  
B. Quantum numbers, degeneracy, and energy levels  
C. Hydrogenic atom wave functions  
D. Multi-electron atoms  
1. 2-electron problem  
2. The self-consistent field method  
3. Electron configurations  
E. Spin-orbit interaction  
F. Total angular momentum  
G. Term symbols for atoms

Chap.12, 13, 14
Chap.15, 18
Chap.20, 21, 22
Mid-Term Exam#2 March 4rd week

IV. Molecular structure
A. The H$_2^+$ molecule
   1. Preliminary considerations
   2. The Schrödinger equation for H$_2^+$
   3. Molecular orbital descriptions for H$_2^+$
B. The variation method
C. Molecular orbitals for homonuclear diatomic molecules
D. Term symbols for diatomic molecules
E. Heteronuclear diatomic molecules
F. Valence bond method
G. Polyatomic molecules
   1. The H$_2$O molecule
   2. The CO$_2$ molecule
H. Delocalized π bonding and the Hückel approximation
I. Computational chemistry

V. Molecular Spectroscopy
A. Energy of molecules
B. Transition probabilities and selection rules
C. Pure rotational spectra
D. Rotational Raman spectra
E. Molecular vibrations
F. Vibration-rotation spectra
G. Electronic transitions
   1. The Franck-Condon principle
   2. Fluorescence and phosphorescence
   3. Lasers

Exam#3 April. Last week

VI. Statistical Thermodynamics
A. The distribution of molecular states
B. The molecular partition function
C. Translational partition function
D. Rotational partition function
E. Vibrational partition function
F. Electronic partition function
G. The total partition function
H. Internal Energy and Entropy
I. The canonical partition function
J. Relationship between the molecular and canonical partition functions
K. Other thermodynamic functions

Final Exam May 5th
## 11 HOMEWORK ASSIGNMENT

<table>
<thead>
<tr>
<th>TOPIC</th>
<th>CHAP.</th>
<th>ASSIGNED PROBLEMS</th>
</tr>
</thead>
<tbody>
<tr>
<td>From Classical to Quantum mechanics</td>
<td>12</td>
<td>Q12.3, Q12.5, Q12.9, Q12.10, Q12.13, Q12.15, Q12.16</td>
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<tr>
<td>The Schrödinger Equation</td>
<td>13</td>
<td>Q13.3, Q13.9, Q13.12, Q13.13, Q13.16, Q13.18, Q13.19, Q13.20</td>
</tr>
</tbody>
</table>

***EXAM I Feb. 3rd week ****

| The Quantum Mechanical Model for Vibration...     | 18    | Q18.2, Q18.3, Q18.7, Q18.12, Q18.13, Q18.15, Q18.18, Q18.201 |
| The Hydrogen Atom                                | 20    | Q20.2, Q20.4, Q20.9, Q20.11, Q20.12, Q20.16, Q20.17, Q20.19 |
| Many-Electron Atoms                              | 21    | Q21.4, Q21.6, Q21.10, Q21.11, Q21.12, Q21.14, Q21.15, Q21.20 |

***EXAM II March 4th week ****

| Quantum States for Many-Electron Atoms           | 22    | Q22.1, Q22.2, Q22.4, Q22.8, Q22.9, Q22.10 |
| The Chemical Bond in Diatomic Molecules          | 23    | Q23.5, Q23.7, Q23.17, Q23.18, Q23.19, Q23.23, Q23.25, Q23.26 |

***EXAM III April Last week****

| Molecular Structure of Polyatomic Molecules      | 24    | TBA |

***FINAL EXAM May 5th****

The text book problems assigned above are identified by the key words below:
Q: discussions questions
P: problems

## 12 TEACHING STRATEGIES

For this course, the basic concepts will be discussed and illustrated with examples and demonstrations, movies, etc whenever possible. Lectures will be delivered using standard blackboard and power point presentations (available through http://blackboard.uncfsu.edu/). I strongly encourage students to read the checklist of key ideas at the end of each chapter in the textbook each time that a new chapter will be started. Students are also encourage to take notes, to ask questions and to participate in class discussions.
13 BIBLIOGRAPHY