

Chemistry 395/437: Quantum Chemistry
Department of Chemistry, Loyola University Chicago
Spring 2018

Instructor: Dr. Dan Killelea
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Office Hours: M 1:30p and by appointment (FH 103)
Class: T Th, 8:30–9:45 am, FH-007
Text: Quantum Chemistry, Donald A. McQuarrie (2nd Ed.)
Course Prerequisites: Chemistry 302 or concurrent registration. If you have not completed the course prerequisite, you may be administratively dropped from the class.

Course Overview

Quantum mechanics is the best model we presently have available for describing the behavior of microscopic (e.g. atomic scale) systems. Developed in the early 1900's, the theory has been essential for understanding many of the scientific advances in the past hundred years, and has enabled a sometimes clear picture of atomic-scale phenomena. A qualitative understanding of quantum is necessary for a chemist, and an understanding of the fundamentals of quantum mechanics is valuable for any chemistry involved with research. Many 'ordinary' techniques in chemistry, for example, absorption of light (spectroscopy), the structure of solids, and semiconductor devices, are all so-called 'quantum' phenomena. In this course we will study the fundamentals of quantum mechanics and how they apply to chemical systems. A key goal will be to de-mystify many of the 'odd' behaviors that have been casually assigned to quantum mechanics.

Course Goals:

- Master fundamental quantum mechanical principles and problem-solving techniques.
- Develop working knowledge of terminology and tools used by quantum chemists.
- Learn how quantum mechanics manifests itself in nature and experimental science.
- Understand advantages and limitations of approximation methods for solving complex problems

Exams, Homework, and Grading

There will be a three hour exams this semester, two during regularly scheduled class periods and the last one during the final exam slot (Saturday, 9:00am – 11:00am, 5 May). There will be no make up exams. Homework will be assigned and collected through the semester, usually assigned on a Tuesday and due the following.

Supplementary Texts

The Principles of Quantum Mechanics, 4th Ed., P.A.M. Dirac

Introduction to Quantum Mechanics, Pauling and Wilson

Introduction to Quantum Mechanics, 2nd Ed., David Griffiths

Physical Chemistry, 2nd Ed., Rice, Ross, and Berry

Grading: The grade will be based on completion of homework and exam scores.

400 Points Total

Exam 1 :	100 points
Exam 2:	100 points
Exam 3 (during final slot):	100 points
Homework:	100 points
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	400 points

Grading Scale:

>85%	A	80-85	A-	75-80	B+
65-75	B	60-65	B-	50-60	C
45-50	D	<45	F		

Schedule

We will not have class 13 Feb, 6 and 8 Mar, and 3 and 5 April.

Tentative Lecture Topics:

"New" Experimental Results and the Birth of the Quantum Theory

Physical and Mathematical Foundations for the Quantum Theory

Classical Mechanics, Complex Variables, Fourier Transforms, Gaussian Functions

The Uncertainty Relationships

The Schrödinger Equation

The Postulates of Quantum Mechanics

Operators, Wavefunctions and Eigenvalue Equations,

Expectation Values, Quantum Measurement

Application of the Schrödinger Equation

Free Particle, Potential Barrier and Particle in a Box Problems

Energy levels, wavefunctions, band structure, tunneling, and wavepackets.

The Simple Harmonic Oscillator, Polynomial Treatment

The Matrix Formulation of Quantum Mechanics

Bras & Kets, Operator Representations, and Matrix Manipulations

Simple Harmonic Oscillator Revisited: Ladder Operators

Angular Momentum, the Hydrogen Atom, and Atomic Orbitals

Quantum Mechanical Treatments of Molecular Bonding: H_2^+ , H_2 , ...

Molecular Orbital Approach, Valence Bond Approach

Approximation Methods

Time Independent Perturbation Theory

Time Dependent Perturbation Theory

Variational Principle

Coupled Harmonic Oscillators

The Anharmonic Oscillator

Academic Integrity

All students in this course are expected to have read and to abide by the demanding standard of personal honesty, drafted by the University, can be viewed at:

https://www.luc.edu/academics/catalog/undergrad/reg_academicintegrity.shtml

The basic commitment of a university is to search for and to communicate the truth as it is honestly perceived. The university could not accomplish its purpose in the absence of this demanding standard. To the extent that this standard is respected, a genuine learning community can exist. Students of this university are called upon to know, to respect, and to practice this standard of personal honesty.

Plagiarism is a serious form of violation of this standard. Plagiarism is the appropriation for gain of ideas, language, or work of another without sufficient public acknowledgement and appropriate citation that the material is not one's own. It is true that every thought probably has been influenced to some degree by the thoughts and actions of others. Such influences can be thought of as affecting the ways we see things and express all thoughts. Plagiarism, however, involves the deliberate taking and use of specific words and ideas of others without proper acknowledgement of the sources.

I have no tolerance whatsoever for cheating or plagiarism. *Any instance of dishonesty (including those detailed on the website provided above or in this syllabus) during a quiz, test, or exam will result in a failing grade for the course.* The Dean of Arts & Sciences and The Chair of The Department of Chemistry & Biochemistry will also be notified. I truly hope to never have to invoke these processes. Please be honest with your work.

Teamwork: I strongly encourage you (the class) to work together to solve assigned and unassigned problems. In order to learn and excel in Physical Chemistry, you should work through problems. The assigned problems are a minimum. Work together with your classmates, if you do not understand something, someone else may. You will also find that explaining a solution to your classmate will cement the information in your mind, and make you a better student.

When working as a group, if each member contributes to the discussion, and you each hand in very similar work, that is perfectly acceptable given the nature of the assignments. On the other hand, if someone simply copies an assignment from someone else, that is plagiarism, and will be treated as such.

Students with Disabilities

If you have any special needs, please let me know in the first week of classes. The university provides services for students with disabilities. Any student who would like to use any of these university services should contact the Services for Students with Disabilities (SSWD), Sullivan Center, (773) 508-3700. Further information is available at <http://www.luc.edu/sswd/>.

Your well-being

If there are events occurring in your life that cause school to diminish in its priority, please discuss this with me or contact the Wellness Center (<http://www.luc.edu/wellness/index.shtml>) or the dean of students (http://www.luc.edu/studentlife/dean_of_students_office.shtml) for assistance. These are services that **your** tuition pays for and can be invaluable for your personal health and maintaining progress towards your degree.