Chemistry 120A - Physical Chemistry

“Quantum Mechanics and Elementary Spectroscopy”

Spring 2025

Course Synopsis

Quantum mechanics is one of the most exciting theories in chemistry and is indispensable for describing the motion and interaction of microscopic particles such as electrons, nucleons, and photons. Part of chemistry’s beauty stems from the hierarchical emergence of structure and dynamics from these particles, governed by the rules of quantum mechanics. Quantum mechanics has arguably had a greater impact on chemistry than any other theory — and it is based on only a handful of postulates! With relatively few mathematical principles, we will construct the quantum mechanical edifice to explain key principles and tools in chemistry, including atomic structure, the nature of chemical bonds, molecular vibrations, computational chemistry, and the interaction of light with matter. The overall goal of this course is to equip you with the knowledge needed to formulate a rigorous quantitative foundation for chemical principles that are otherwise merely observational. Additionally, we will explore how quantum principles function in the context of their most recent applications, such as coherent (wavelike) phenomena and the interaction of quantum light (entangled photons) with matter—topics that lie at the cutting edge of research.

Lectures: M,W,F 11:10 AM – 11:59 PM, 120 Latimer

Discussion: M,T 7:00 – 8:30 PM, 425 Latimer (except when announced otherwise on bCourses).

Instructors:

Professor Hendrik Utzat

Email: hutzat@berkeley.edu

231 Hildebrand Hall

Professorial office hours: M 3:30-4:30, W 4-5 PM PM, in Hildebrand Hall 231.

Graduate Student Instructors

GSI Bokang Hou, bkhou@berkeley.edu (he/him/his)	Office hours: 5-6 pm Thursday, 4-5 pm Friday Lewis 1
GSI Tommy Lin, tommy_lin@berkeley.edu (he/him/his)	Office hours: 4-5 pm Monday, 9-10 am Friday Lewis 1

Students who are unable to make office hours but who need to meet with one of the Graduate Student Instructors (GSIs) for course-related issues should contact GSIs by email.

Course grading

Problem sets will be assigned for homework; approximately nine homework sets for the entire semester. This number may be reduced in case of TA labor strikes. Specific dates for assignments and examinations will be announced by the instructors and can change and will be announced on bCourses.See additional policy regarding homework scoring and missed homework below.

There will be two in-class midterm examinations (50 minutes, on Feb. 28, 2025 and April. 7, 2025), and a final examination (180 minutes, Tue, May 13 • 7:00P - 10:00P • Exam Location TBD). Grades will be based upon scores on homework (normalized to 100 points total, counts 20%), midterms (2 exams, 100 points each, counts 40% total), and the final examination (200 points, 40%) = total 500 points (100%).

Filling out the course evaluations at the end of the course will count as a bonus of 1%, or 5 points. Your feedback will actually make a difference and further improve the learning experience of future cohorts.

Midterms and Final Exam

There will be no makeup exams. If a midterm is missed for a medical or other valid reason and approved by the instructors, a score will be calculated based on the other completed examination scores (not the homework). For this to apply, students must (1) email the instructor before the start of the exam, and (2) present a doctor's note. A missed final exam or two missed midterms will result in an 'incomplete' grade.

Honor Code

Your grade in this class shall reflect your honest effort and knowledge of the basics of quantum mechanics. Collaboration between students in working on homework assignments is encouraged, but copying of solutions (and their mistakes) is not allowed. Use of large language models may help for self-study, but querying for explicit help with homework is not permitted.

Accommodations

If you have DSP accommodations for this class, please work with the DSP office and, additionally, inform both TAs and the professor in an email of your accommodations. Please do this within the first two weeks after the start of instruction.

Course Websites

If you are enrolled for this class, you will automatically be given access to the bCourses site (Physical Chemistry 120A, Spring 2025). All course materials (problem sets, solutions, and any supplemental materials) as well as all announcements will be posted on the bCourses site.

Course Capture

We have included the course in the Spring 2025 Course Capture program. Course recordings will be automatically posted to bCourses, on the Class Page for Chem 120A. Course Capture is not controlled by the instructors and some lectures may not be recorded due to technical problems.

Lectures and Discussion Sections: Lectures are scheduled on Monday, Wednesday, and Friday at 11:00 AM in 120 Latimer Hall. We also offer optional Discussion Sessions held on Mondays (in 425 Latimer) and Tuesday (in 425 Latimer) evenings from 7:00 PM to 8:30 PM. NOTE: We will not offer discussion in some weeks, which will always be announced on bCourses.

Homework Policy

- Any questions regarding homework must first be directed to the GSIs.

- There will be approximately 9 homework assignments.
- Some, but not all problems on a given problem set will be graded to establish a grade for the homework.
- One out of approximately 9 homework assignments will be dropped in the final calculation of the homework grade. If students can't complete the homework for health reasons, the one-drop policy still applies. We encourage handing in all homework assignments unless you absolutely can't. If homework is not handed in, a grade of zero will apply for that problem set.
- Working together on homework assignments is encouraged, but every student needs to turn in their own homework. Copying solutions is not permitted.
- Late homework will be accepted up to 24 hours after the assignment due date and without extension request. After that, no credit will be given for late homework.

Textbooks and Reading Assignments

The textbook for the course is

- W. Atkins & R. S. Friedman, *Molecular Quantum Mechanics 5th Edition* (Oxford University Press, Oxford, 2010).

Reading assignments from this book are given in the Lecture Outline and Schedule. Additional readings from other texts are suggested. These other texts include:

- McQuarrie, Quantum Chemistry, 2nd Edition (University Science Books, 2008); the same chapter material is fully contained in McQuarrie and Simon, Physical Chemistry: A Molecular Approach.

and further:

- Ira N. Levine, *Quantum Chemistry*, (Prentice Hall; 7th edition, February 16, 2013),
- Eugen Merzbacher, *Quantum Mechanics*, (Wiley; 3rd edition, 2013),
- Ira N. Levine, *Molecular Spectroscopy*, (Wiley, April 1975),
- M. Barrow, *Molecular Spectroscopy*, (McGraw-Hill, International Edition, 1988).

Provisional Lecture Outline and Schedule

The below topical outline is an approximate guidance and is subject to adaptations during the semester.

Chemistry 120A Spring 2025,
Professor Hendrik Utzat

Date	Instructor	Lecture #	Topics	Further Reading
I. Introduction and the Schroedinger equation				
22-Jan	HU	1	Intro / Motivation for quantum	Atkins Intro, Chap 1 McQuarrie Chap 1, Math A
24-Jan	HU	2		
II. The Q.M. formalism and analytically exact model systems				
27-Jan	HU	3	Postulates, linear operators, and properties of the Schroedinger equation	Atkins 1.1-1.14, McQuarrie 4.1-4.6
29-Jan	HU	4		
31-Jan	HU	5		
3-Feb	HU	6	Particle in 1D box, superposition and dynamics	Atkins 2.10-2.11, McQuarrie 3.1-3.8
5-Feb	HU	7		
7-Feb	HU	8	particle in 3D box, degeneracy	Atkins 2.12-2.13, McQuarrie 3.9
10-Feb	HU	9	Quantum Harmonic Oscillator	Atkins 2.14-2.16 and 2.1-2.4, McQuarrie 5.1-5.5
12-Feb	HU	10		
14-Feb	HU	11	Particle on a ring	Atkins 3.1-3.4
III. Electron in atoms and atomic orbitals				
17-Feb	HU	-	No Class	

19-Feb	HU	12	Spherical Harmonics Angular momentum	Atkins 3.6-3.9 McQuarrie 5.8-5.9
21-Feb	HU	13	Spherical Harmonics Angular momentum	Atkins 3.6-3.9 McQuarrie 5.8-5.9
24-Feb	HU	14	Rigid Rotor	Atkins 3.6-3.9 McQuarrie 5.8-5.9
26-Feb	HU	15	Hydrogen Atom	Atkins 3.11-3.16, McQuarrie 6.1-6.6
28-Feb	**HU**	**15**	**First midterm in class (up to and including rigid rotor)**	
3-Mar	HU	17	Helium atom	Atkins 7.8, McQuarrie 6.7
5-Mar	HU	18		
7-Mar	HU	19	Perturbation theory: first and second order, degenerate perturbation theory; application to helium atom	Atkins 6.1-6.4, McQuarrie 7.4
10-Mar	HU	20		
12-Mar	HU	21	Variational principle, Secular equation, variational principle in orthogonal basis; application to helium atom.	Atkins 6.5-6.6, McQuarrie 7.1-7.3
14-Mar	HU	22	Stern Gerlach experiment, spin angular momentum	Atkins 4.8, 7.11-7.24, McQuarrie 8.3-8.6
17-Mar	HU	23	Spin statistics, Pauli principle and Slater determinants, spin functions.	Atkins 4.8, 7.11-7.24, McQuarrie 8.3-8.6
19-Mar	HU	24		Atkins 4.8, 7.11-7.24, McQuarrie 8.3-8.6

21-Mar	HU	25	Helium excited states, singlet and triplet	Atkins 7.9-7.10, 7.12-7.15, McQuarrie 8.1-8.2
31-Mar	HU	26	Lithium atom, Born-Oppenheimer approximation I	Atkins 7.9-7.10, 7.12-7.15, McQuarrie 8.1-8.2 & Atkins 8.1, McQuarrie 9.1
2-Apr	HU	27	Born-Oppenheimer approximation II	Atkins 7.9-7.10, 7.12-7.15, McQuarrie 8.1-8.2 & Atkins 8.1, McQuarrie 9.1
IV. Interatomic Interactions and Chemical Bonding				
4-Apr	HU	28	Chemical Bond I: H2+	Atkins 8.2, McQuarrie 9.2-9.5
7-Apr	**HU**	**29**	**Second midterm in class (up to and including BO approximation)**	
9-Apr	HU	30	Chemical Bond II: H2 and molecular orbital theory	Atkins 8.4-8.5, 11.1, McQuarrie 9.6-9.9
11-Apr	HU	31	Chemical Bond III: Homonuclear and heteronuclear diatomic molecules, Hund's rules	Atkins 8.4-8.5, 11.1, McQuarrie 9.6-9.9
14-Apr	HU	32	Polyatomic molecules + Huckel theory for conjugated molecules	Atkins 8.7, 10.1-10.3 + Atkins 8.8, McQuarrie 10.5-10.6
V. Time-dependent perturbation of quantum states and elementary spectroscopy				

16-Apr	HU	33	Time-dependent perturbation theory, spectroscopic transitions	Atkins 6.7-6.11, Atkins 10.1, McQuarrie 13.11
18-Apr	HU	34		Atkins 6.7-6.11, Atkins 10.1, McQuarrie 13.11
21-Apr	TBD	35	Special Topic: Computational Chemistry (not part of final exam)	Selected uploaded resources
23-Apr	TBD	36	Special Topic: Computational Chemistry (not part of final exam)	Selected uploaded resources
25-Apr	HU	37	Rotational spectra, rigid rotor, nuclear spin	Atkins 10.3-10.6, McQuarrie 13.2, 13.4, 13.8, 13.12
28-Apr	HU	38	Vibrational spectra, harmonic and anharmonic models, Rotational-vibrational spectra	Atkins 10.7-10.13, McQuarrie 13.2 13.5, 13.13
30-Apr	HU	39	Electronic transitions, Franck-Condon principle	Atkins 6.9, Atkins 11.4-11.16 McQuarrie 13.6-13.7
02-May	HU	40	Special Topic: Quantum optics for chemists (not part of the final exam)	Selected uploaded resources from Mark Fox: Quantum Optics, Oxford.

Final Exam: Tue, May 13 • 7:00P - 10:00P •(time for DSP students tbd), Exam Location TBD