Chemistry 6491: Quantum Mechanics

Fall 2026

Course Information

Location:	Klauss 1447
Time:	MWF 9:30 - 10:20 am
Course website:	Through Canvas

Instructor

Instructor:	Prof. Joshua Kretchmer
Email:	jkretchmer@gatech.edu
Office:	MoSE 2100H
Office Hours:	TBD

Office hours will be held in person in my office if there are only a couple of students. If a larger number of students show up to office hours we will move to a larger classroom and I will leave a note on the door to my office.

Course Description

This course will cover important concepts and applications of quantum mechanics at the intermediate level to provide a strong foundation for research in physical chemistry. A strong focus will be on the mathematical underpinnings of quantum mechanics as well as how concepts and techniques connect to modern research.

Course Goals and Learning Outcomes

- The ability to solve the common back-of-the-envelope problems that appear in physical chemistry research
- The ability to discuss concepts with researchers in quantum mechanics across fields
- A sufficient background in the fundamentals of quantum mechanics to learn more complex concepts

Requirements and Grading Scheme

Problem sets	15%
Quizzes	15%
Midterm	30%
Final	40%

Description of Graded Components

Problem sets are take-home assignments associated with the course lecture material and textbook content. Students are free to use their class notes, the textbook, and other references to help complete the problem sets. Students are additionally encouraged to collaborate with each other, but each student should turn a completed assignment that reflects their own work. Problem sets will be assigned on a 1-1.5 weekly basis. The exact time-frame may fluctuate depending on the pacing of course material given the amount of discussion in class. This ensures that the problem sets stay in sync with the course content. Paper copies of the completed problem sets should be turned in at the beginning of lecture on the due date. Extensions on problem sets can be requested due to illness, approved institute activities, or other unforeseen circumstances, but must be requested at least 24 hours prior to the deadline. Late problem sets will not be accepted without an approved extension.

The problem sets will be graded purely in terms of completion, not based on accuracy. If you make a legitimate attempt on each problem, you will be awarded full points for the problem set. The solution set for all problems will be posted online to canvas following the deadline. The motivation for this choice is that problem sets are meant to be an opportunity for students to struggle and think critically about the material. I do not want students focused on obtaining the correct answer as quickly as possible just to ensure they obtain a high accuracy grade on the problem sets.

Coupled with the problem sets, the course will involve a set of in-class quizzes. Quizzes will be strongly coupled to a given problem set and involve a short question to test students' knowledge of the material from the previous problem set. Quizzes will take place one or two class periods after the deadline for the corresponding problem set. The quizzes will take place during lecture time and should not take more than 5-10 minutes. The purpose of the in-class quizzes is to provide students with feedback throughout the semester on how well they understand the material.

The course will involve one midterm exam and one final exam. The midterm exam will be given during the 50 minute lecture time and will be fully closed book. However, the exam will include a cover sheet of important reference equations. The exam is expected to be completed within the 50 minute block of time. The final exam will follow the same structure, but will be given during the 2 hour and 50 minute final exam block. In comparison to the quizzes, these exams will be less tied directly to the problems on the problem sets and instead test extensions of the concepts presented on the problem sets.

Auditors are required to attend a minimum of 1/2 of the lectures, unless other accommodations are discussed with the instructor. Pass/fail students are required to take both exams and the final and receive an overall passing grade.

Grading Scale

Your final grade will be assigned as a letter grade according to the following scale, though grade thresholds may be adjusted down (but not up) at the end of the semester, as determined by the instructor.

A 85-100 %
B 70-85 %
C 55-70 %
D 40-55 %
F 0-40 %

Required Textbook

R. Shankar, *Principles of Quantum Mechanics*, 2nd ed. (Plenum, New York, 1994).

Other Books that may be Helpful

Introductory Texts

- D. A. McQuarrie, *Quantum Chemistry* (University Science Books, Mill Valley, CA, 1983).
- D. J. Griffiths, *Introduction to Quantum Mechanics* (Pearson Prentice Hall, Upper Saddle River, NJ, 2005).
- P. Atkins and R. Friedman, *Molecular Quantum Mechanics* (Oxford University Press, Great Clarendon St, Oxford, 2005).

Advanced Texts

- E. Merzbacher, *Quantum Mechanics*, 3rd ed. (Wiley, New York, 1998).
- C. Cohen-Tannoudji, B. Diue, and F. Laloë *Quantum Mechanics*, 3rd ed. (Wiley, New York, 1977).
- Szabo and N. S. Ostlund, *Introduction to Advanced Electronic Structure Theory* (Dover Publications Inc., Mineola, NY, 1996).

Topics

Unit I: Fundamentals of Quantum Mechanics

(A) Introduction to quantum mechanics:
- Double slit experiment
- De Broglie wavelength
- The Schrödinger equation

(B) Mathematical Background:
- Linear vector spaces
- Dirac notation
- Operators

(C) Postulates of Quantum Mechanics

(D) Model problems:
- 2-state system
- Particle in a box
- Free particle
- Harmonic oscillator

(E) The classical limit: Ehrenfest's theorem

(F) Angular momentum:
- Spherical harmonics
- Ladder operators
- Rigid rotator and rotational spectroscopy

(G) The Hydrogen atom

Unit II: Advanced Fundamentals

(A) Spin

(B) Addition of angular momenta

(C) Multi-particle systems

Unit III: Approximate Methods

(A) Variational method:

- Variational theorem
- Equivalence of Raleigh-Ritz procedure and diagonalization

(B) Time-independent perturbation theory

Unit IV: Possible Advanced Topics

(A) Time-dependent perturbation theory

(B) Interaction of light with matter

(C) Time-dependent density matrix and the interaction picture

(D) Path-integrals

Course Policies, Expectations & Guidelines

Academic Integrity:

Georgia Tech aims to cultivate a community based on trust, academic integrity, and honor. Students are expected to act according to the highest ethical standards. For information on Georgia Tech's Academic Honor Code, please visit https://catalog.gatech.edu/policies/honor-code/ or https://catalog.gatech.edu/rules/18/.
Any student suspected of cheating or plagiarizing on a quiz, exam, or assignment will be reported to the Office of Student Integrity, who will investigate the incident and identify the appropriate penalty for violations.

Accommodations for Students with Disabilities:

If you are a student with learning needs that require special accommodation, contact the Office of Disability Services at (404) 894-2563 or http://disabilityservices.gatech.edu/, as soon as possible, to make an appointment to discuss your special needs and to obtain an accommodations letter. Please also e-mail me as soon as possible to set up a time to discuss your learning needs.

Collaboration, Group Work, and Use of Generative AI:

Students are allowed to discuss problem sets together, but should turn in assignments that reflect their own work. Students will not be allowed any collaboration on exams. Part of the course work in this class will involve solving complicated mathematical problems that in principle generative AI will be able to solve on your behalf. However, *(i)* if you rely on generative AI you will not succeed in the course and *(ii)* you will not accomplish the course goals of having a sufficient understanding of quantum mechanics to successfully participate in

research in physical chemistry. Consequently, I expect students to avoid using generative AI as much as possible to directly solve problems on the problem set. Instead, I strongly encourage students to come to office hours if you are struggling with the problems.

Student-Faculty Expectations Agreement:

At Georgia Tech we believe that it is important to strive for an atmosphere of mutual respect, acknowledgement, and responsibility between faculty members and the student body. See http://www.catalog.gatech.edu/rules/22/ for an articulation of some basic expectations that you can have of me and that I have of you. In the end, simple respect for knowledge, hard work, and cordial interactions will help build the environment we seek. Therefore, I encourage you to remain committed to the ideals of Georgia Tech while in this class.

Campus Resources for Students:

A list of resources for graduate students is given on the Office of Graduate and Postdoctoral Education website, which can be found at https://gradpostdoc.gatech.edu/ or https://grad.gatech.edu/current-students. Specific information for current graduate students includes:

- Academic resources such as the Communications Center, Language Institute, Library, Catalog, Registrar, resources for conducting research, Advocacy and Conflict Resolution resources, and how to manage unexpected situations that may impact your academic performance. For more information about these resources, please visit https://grad.gatech.edu/academic-resources.

- Student resources such as Campus Services, Child Care/Family programs, Health and Wellness, Career Services, and the Student Resource Guide. For more information about these resources, please visit https://grad.gatech.edu/student-resources

- Professional development such as the programming from the Career Center and other professional development resources and events. For more information about these resources, please visit https://grad.gatech.edu/career-development.

Student Well-Being

At Georgia Tech, we are concerned about your overall physical, social, and mental well-being. This is especially true for new graduate students as the transition from undergraduate to graduate education and research can be daunting. A comprehensive list of wellness related resources has been compiled and maintained by the Office of the Vice President for Student Engagement and Well-being. For more information about these resources please visit, https://students.gatech.edu/student-resource-guide.

More resources on supporting student well-being on the syllabus and beyond are available through the Learning Well Initiative. For more information about these resources please visit,\\ https://blog.ctl.gatech.edu/2025/07/21/supporting-student-success-through-the-learning-well-initiative/.