Syllabus for Chemistry 8541: “Dynamics”
Fall Semester 2022, four credits

11:15–12:30 Mon & Fri (Fri. 9/9/2022 – Mon. 12/12/2022)

Instructor: Donald G. Truhlar
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TA: none

Prerequisite: Undergraduate physical chemistry course

Format of the class:
This course is scheduled as a remote synchronous course. In particular, this class will meet by zoom on Mondays and Fridays from 11:15 am to 12:30 pm, starting Friday Sept. 9 and continuing through Monday December 12.

Holiday: Friday Nov. 25 is a University holiday; there will be no class that day.

Textbook:

*Modern Classical Mechanics*
by T. M. Helliwell and V. V. Sahakian
Publisher: Cambridge University Press
doi.org/10.1017/9781108874687
required? yes

Description and scope of the course:

Chemistry 8541 is a graduate course in physical chemistry and chemical physics. The course has two topics. One topic is the mathematics of chemical physics. The other topic is classical mechanics and classical dynamics, including Newtonian, Lagrangian, and Hamiltonian dynamics. We cover mathematics not just because of its importance in classical dynamics, but also because the mathematics covered is the mathematics that every physical Chemistry or Chemical Physics Ph.D. should know. We cover classical dynamics not just because of its importance in its own right, which is considerable, but also because understanding of classical dynamics provides a solid foundation for understanding many parts of quantum mechanics and statistical mechanics. The mathematical topics chosen for coverage are the ones most useful for physical chemistry and chemical physics, and much of the math we cover is also useful for quantum mechanics, statistical mechanics, and spectroscopy. The course is focused on practical mathematics and practical classical mechanics, not on formal developments and proofs.

I have selected a textbook that has some brief reviews of some of the mathematics; I will present additional mathematical background in the lectures as needed. Students are also
encouraged to broaden their understanding by consulting other books; those on the reading list at the end of this document are especially recommended.

Objective of the course

To give the student the level of understanding of mathematical methods and classical dynamics that is a foundation for large parts of chemical dynamics, quantum mechanics, molecular spectroscopy, chemical kinetics, materials science, and statistical mechanics. The textbook includes an introduction to relativity; I will minimize attention on that and focus on nonrelativistic classical dynamics.

Class participation

The class will be taught in a participatory style emphasizing class discussion (online) and class participation (online). Ordinarily we will all have our cameras on to facilitate communication. I recommend having an application that allows you to share your screen with the class.

Class preparation

Students should prepare for each class by reading the assigned material prior to the class period. Come to class prepared to discuss the material. Have the textbook handy during class so we can refer to it if desired. The material for the next class will be announced at the end of each class. Sometimes there will also be homework.

Class organization

I have now taught this course several times, and each time it is different. Most years I have had two textbooks – one for math and one for dynamics, and every year I changed at least one of the textbooks and the order of coverage. This year I again have a new textbook, and it is a single textbook. This is a book I have never used before. The reason I change textbooks every year is to keep the course fresh. No textbook has everything we need, so we will cover some material, especially mathematical background, that is not in the textbook.

What is the difference between a graduate class and simply reading a good book on the subject (or checking out a good Web site or tuning in to a set of online asynchronous lectures)? The answer I came up with is real-time, in-person student participation, and current research into learning is coming to the same conclusion. We have always had a lot of student participation in this course, and this year we will try for even more, via the interactive nature of Zoom. There are many good books and good Web sites on almost any topic in mathematics or classical dynamics; students are encouraged to learn from all available sources. But in class, I want to do more than present a lecture to a passive audience.

Usually the material will be covered in class differently than in the reading. I view classes as complementing the reading – this usually means not repeating the same material in the same way. And yet I want class participation, so we will also discuss the material in the textbook that students should come prepared to discuss. We will try to balance discussion of the text material with new perspectives.
Presentations

In addition to active participation in every class, students will assist in presenting the material and in some cases they will be assigned sections of the material to present to the class. Class participation by the whole class is encouraged for every class, no matter who is leading a particular segment.

Grading

For an explanation of the University grading system please see http://policy.umn.edu/education/gradingtranscripts

The two major grading systems used are A-F and S-N. The present course uses the A–F system.

Different students come in with different backgrounds. Everybody will advance in understanding at a different rate. That’s expected in graduate school. Therefore grades will not be based on learning a set amount of material, but rather on full participation in the learning experience.

Grades will be based entirely on class participation and homework, with the emphasis being class participation; there will be no written or oral exams.

Making up for absences

Absences may occur due to unavoidable or legitimate circumstances. Such circumstances include illness, emergencies, subpoenas, jury duty, military service, bereavement, and religious observances. For complete information, please see:

http://policy.umn.edu/education/makeupwork.

If a class is to be missed, please notify the instructor in advance, when possible. If a class is missed, the makeup assignment is to hand in a three-page PDF summary of the assigned material for that class; this is due one week after the missed class.

Electronic copies of information

Copies of this syllabus, including the reading list at the end, are available at

https://truhlar.chem.umn.edu/courses/chemistry-8541-dynamics
Students with disabilities
Students with disabilities that affect their ability to participate fully in class or to meet all course requirements can arrange reasonable accommodations through the Office of Disability Services (612-626-1333). Students who have concerns about disabilities should notify the lecturer and contact that office within the first week of class.

Student conduct and responsibilities
University policies on student conduct and responsibilities may be found at:
  http://policy.umn.edu/education/studentresp
  https://regents.umn.edu/sites/regents.umn.edu/files/policies/Sexual_Harassment_Sexual_Assault_Stalking_Relationship_Violence.pdf

Equity, diversity, equal opportunity, and affirmative action
The University provides equal access to and opportunity in its programs and facilities, without regard to race, color, creed, religion, national origin, gender, age, marital status, disability, public assistance status, veteran status, sexual orientation, gender identity, or gender expression. For more information, please consult Board of Regents Policy:

Mental health and stress management
Students may experience a range of issues that can cause barriers to learning, such as strained relationships, increased anxiety, alcohol/drug problems, feeling down, difficulty concentrating, and/or lack of motivation. These mental health concerns or stressful events may lead to diminished academic performance and may reduce a student’s ability to participate in daily activities. University of Minnesota services are available to assist with such issues. More information about the broad range of confidential mental health services available on campus may be found on via the Student Mental Health Website:
READING LIST, IN ADDITION TO THE TEXT BOOK

The classics:

Classical dynamics

“Classical Mechanics,” 3rd edition, H. Goldstein, C. Poole, J. Safko; Addison Wesley, San Francisco, 2002. Older editions are just as good; the 2nd edition may even be better.


Mathematics

"Methods of Theoretical Physics," P. M. Morse and H. Feshbach; McGraw-Hill, New York, 1953. (two volumes) (not as broad coverage as the other books)


Recommended textbooks for supplemental reading:

Classical dynamics


Mathematics


