Syllabus for Chemistry 8541: "Dynamics"
Fall Semester 2018, four credits

11:15–12:30 Mon Fri (Fri. 9/7/2018 – Mon. 12/10/2018) 283 Kolthoff

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Office hours: usually available after lectures
Preferred method of contact: in person

TA: none

Prerequisite:
Undergraduate physical chemistry course

Description and scope of the course:
Chemistry 8541 is a core 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 mechanics, but because the mathematics covered is the mathematics that every physical chemistry or chemical physics Ph.D. should know. We cover classical mechanics not just because of its importance in its own right, but also because understanding of classical mechanics provides a solid foundation for understanding quantum mechanics and some parts of statistical mechanics.

Mathematical principles will be illustrated with physical examples when possible. More significantly though, the mathematical topics chosen for coverage are the one most useful for physical chemistry and chemical physics. The course is focused on practical mathematics and practical classical mechanics, not on formal developments and proofs.

I have selected textbooks that, taken together, comprise a balanced combination of topics. Both books are useful reference books for the shelf of a practicing physical chemist or chemical physicist. Each class period will cover material in or similar to a prescribed portion of one or another of the textbooks (often a chapter), as indicated on the schedule. Students are also encouraged to broaden their understanding by consulting other books; those on the reading list are especially recommended.

Textbooks (required)
1. "Mathematical Methods for Scientists and Engineers," Donald A. McQuarrie
    - ISBN 1-891389-24-6 (cloth cover)
    - ISBN 1-891389-29-7 (soft cover)
2. "Classical Mechanics: Systems of Particles and Hamiltonian Dynamics," 2nd ed., Walter Griener
    - ISBN: 978-3-642-03433-6 (paperback)
    - e-ISBN: 978-3-642-03434-3

Other reading
See separate document for recommendations for other reading.

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 quantum mechanics, molecular spectroscopy, chemical kinetics, chemical dynamics, materials science, and statistical mechanics.

Class participation
The class will be taught in an experimental style emphasizing class discussion and class participation. We have tried this in previous years, but this year I will experiment to try to improve the learning experience. Sometimes experiments don't work out; let's hope for the best.

Class preparation
Students should prepare for each class accordingly by
- reading the assigned material prior to the class period
- doing the homework (usually one problem per class, due at the start of the period)

Homework and class preparation may be done in groups, if desired.

Class organization
I have now taught this course several times, and each time it is different. Every year I change at least one of the textbooks and the order of coverage. My goal for this constant changing of the course is to keep the presentation fresher.

Furthermore, I have given a lot of thought to the question: 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 an on-line course)? The answer I came up with is face-to-face 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. Auditors are not allowed in unless they agree to fully participate, so everybody in the room is in the same boat—learning together. 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.

Often the material will be covered in class differently or in a different order than in the reading. I view classes as complementing the reading – this usually means not repeating the same material in the same way.

Presentations
In addition to active participation in every class, students will assist in presenting the material and in the later part of the course, they will be assigned sections of the material to present. In particular, the current plan is that students will lead the last few lectures; assignments for these lectures will be made a few weeks in advance of the student-led lecture periods.

Student presentations can involve one or more of the following: presentation of selected aspects of the assigned material, discussion of the relation of the material to material covered earlier in the course, provision of extra details or insight into derivations or additional perspective, and/or working one or more problems. Class participation by the whole class is encouraged for every class, no matter who is leading.

Written examinations
A written mid-term examination in October and/or a final written examination in December will be scheduled *if class participation is insufficient to gauge the progress of the class*. If class participation is good, which is the preferred alternative, grades will be based entirely on (i) class participation, (ii) homework, and (iii) student-led presentations – equally weighted, 1/3 each.

Every year I warn that there might be surprise quizzes, but usually we do not have any. But one of these days ....

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 A–F.

Different students come in with different backgrounds. Everybody will advance in understanding at a different rate. That's expected; that's graduate school. So grades will not be based on learning a set amount of material. If class participation is sufficiently high, final grades will be based on class participation, homework, and presentations. The lecturer will provide preliminary feedback to the class in October. If class participation is insufficient to gauge the progress of the students, there may be one or two written examinations (see above); if such examinations are scheduled, their percentage contribution to the grade will be announced when they are scheduled.

Lecture schedule
See separate document, which will be updated as the class proceeds.

Holiday
Friday, November 23, which is the day after Thanksgiving.

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, but do not include voting. For complete information, please see:

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

If a class is to be missed, please notify the lecturer in advance, if possible. It a class is missed, the makeup assignment is to hand in the assigned homework and a three-page summary of the assigned material for that lecture; this is due one week after the missed lecture.

Electronic copies of information
Extra copies of the syllabus and reading list are available at

http://truhlar.chem.umn.edu/courses/chemistry-8541-dynamics-fall-2018

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.

Academic dishonesty
Scholastic dishonesty is discussed under the College of Science and Engineering scholastic policies. According to the CLA Classroom Grading and Examination Procedures, scholastic dishonesty is defined as "any act by a student which misrepresents the student's own academic work or that compromises the academic work of another. Scholastic dishonesty includes (but is not necessarily limited to) cheating on assignments or examinations; plagiarizing, i.e., misrepresenting as one's own work any work done by another; submitting the same paper, or substantially similar papers, to meet the requirements of more than one course without the approval and consent of all instructors concerned; depriving another of necessary course materials; or sabotaging another's work."

Student conduct and responsibilities
University policies on student conduct and responsibilities may be found at:

http://regents.umn.edu/sites/regents.umn.edu/files/policies/Student_Conduct_Code.pdf.
http://policy.umn.edu/education/studentresp
https://regents.umn.edu/sites/regents.umn.edu/files/policies/Sexual_Harassment_Sexual_Assault_Stalking_Relationship_Violence.pdf

Students may use personal electronic devices in the classroom for course-related purposes provided the usage is nondisruptive.

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: http://regents.umn.edu/sites/regents.umn.edu/files/policies/Equity_Diversity_EO_AA.pdf.

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:

http://www.mentalhealth.umn.edu.