Syllabus for Chemistry 8541: "Dynamics"
Fall Semester 2017, four credits

11:15–12:30, Mon, Fri (Fri., 9/8/2016 – Mon., 12/11/2016), 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.

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.

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 will cover a prescribed portion of one or another of the books (often a chapter), as indicated on the schedule. Students are also encouraged to broaden their understanding by consulting other books, especially those on the reading list.

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," John R. Taylor (University Science Books, 2005).
    - ISBN-10: 1-891389-22-X
    - ISBN-13: 978-891389-22-1
    - ebook: http://www.uscibooks.com/taylor2.htm

Other reading:
See separate document for recommendations for other reading.

Objectives 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 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. I hope this constant changing of the course keeps 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 a massive open 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, many good books and good Web sites on almost any topic in physical mathematics or classical dynamics; students are encouraged to read widely and maybe even buy a second mathematics reference and a second classical mechanics reference. But in class, we will do more than passively absorb a lecture, since a real-time lecture would be hard pressed to be as clear as a good book.

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 it will be done differently with further experimentation to try to improve the learning experience. Sometimes experiments don't work out; let's hope for the best. Students should prepare for each class accordingly by *reading the material prior to the class period*, doing the homework, and coming to class well prepared

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

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 last few lectures will be led by students; assignments for these lectures will be made a few weeks in advance of the student-led lecture periods.

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, grades will be based entirely on class participation and homework.

Grading:
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. Final grades will be based on class participation and homework if class participation is sufficiently high. Preliminary feedback to the class will be provided by the lecturer 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. I hope the students will participate and try to make the experimental style of teaching work so that everybody gets a good grade and so that we can skip the written exams. Every year I threaten that there might be surprise quizzes, but usually we do not have any. But one of these days ....

Student-led lecture periods:
Student-led lecture periods can involve theoretical lectures on principles and/or discussion of the assigned material in one or more of the following ways: presentation of selected aspects, 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.

Incompletes:
Registered students who do not complete the course will ordinarily receive a failing grade unless they officially withdraw from the course. Incompletes will be given only when discussed with and approved by the instructor before the end of the semester.

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 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."

Lecture schedule:
See separate document.

Holiday:
Fri., Nov. 24: Day after Thanksgiving

Information:
Extra copies of the syllabus, reading list, and schedule are available at

http://truhlar.chem.umn.edu/courses