Fall 2020 - CHEM 590
"Special Topics in Physical Chemistry: Quantum Dynamics"

WHO

Prof. David Beratan
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WHERE

Meeting dates: August 18 - November 12, 2012
Meeting time: Tues. & Thurs., 5:15-6:30 pm via Zoom. The meeting time may be adjusted as fall teaching schedules adapt to COVID-19. The course will be delivered via Zoom.

WHAT

This course is aimed at beginning graduate students (and advanced undergraduates) who have had an introduction to time-independent quantum mechanics and are comfortable with multi-variable calculus and linear algebra.

The course addresses the time-evolution of molecular systems, exploring their dynamics in isolation and in the condensed phase. The framework for understanding systems of this kind involves the time-dependent Schrödinger equation, the quantum Liouville equation, density matrix methods, time-correlation functions, descriptions of system-bath interactions, semiclassical dynamics, and quantum coherence.

As we develop the frameworks for time-dependent quantum mechanics, we will study selected applications in chemistry, drawn from spectroscopy, reaction dynamics, and transport phenomena.

Course materials will be drawn from multiple textbooks and online materials. The course will involve homework assignments and an end-of-term team project that will be written up and presented to the class.

HOW

This class will be "semi-flipped" compared to traditional lecture courses. This means that much of the in-class time will be devoted to discussing conceptual issues and problems, rather than deriving equations. It will be essential that you work through the relevant sections of our homegrown text/self-guided tutorial, along with the assigned readings **in advance of the class meetings** so that you may engage in the classroom activities. **You should set aside 2-3 hours of preparation time for reading and study prior to each class, and should budget a similar amount of time after each class to complete problems that were begun in class.**

Your "Hitchhiker's Guide to the Galaxy" for this course is a developing text/workbook that summarizes the key principles and poses model or "toy" problems that reveal key principles. Please plan to have access to a laptop or desktop during the class and come prepared for active participation. Class time will likely be used in the following way: ~15 min of discussion on the readings; ~50 min devoted to group problem solving and explorations, using Python as well as pencil and paper, and ~10 min of summary discussion to wind things up at the end of class, including a summary of open questions, challenges, and points of confusion.

Computation. This year, we will use Jupyter notebooks with Python to solve model problems.

GRADING

- Class participation, preparation, and team engagement (33%)
- Homework: one assignment per unit (33%)
- Term project and presentation (33%) Student projects may include explorations of: quantum computing; fluctuation theorems, correlations functions; debates surrounding classical and quantum coherences in chemistry/biochemistry; signatures of electronic vs vibronic coherences; the quantum - stat mech interface.

INTEGRITY

- Projects conducted within the classroom as well as homework assignments are intended to be discussed and worked on intensively in groups. While discussion is essential, you must write your own computer programs and write up the homework solutions independently. To be specific, you may discuss your strategies extensively, sharing ideas and tricks, but you may not "copy and paste" the work of others. Similarly, you may not divide the homework among members of the class and simply pool your efforts without pitching in on every problem.
- With respect to attribution of the work of others in your team project, please consult the Duke Library resource on plagiarism: http://library.duke.edu/research/plagiarism/index.html

The course is 13 weeks long: August 18 – November 12

Course Content:

Unit #0: Introduction to our course and teaching a project oriented/hands on course in the times of COVID-19; What I wish I had learned about quantum mechanics earlier in life; Discussion of open questions in our field; Introduction to Jupyter notebooks and Python (Mr. Valdiviezo) (2 weeks)

Unit #1: Introduction and time-dependent Schrödinger equation; propagation in time; two- and many-level systems. Real and imaginary Hamiltonians. Kinetic master equations vs quantum dynamics for few state systems. Multi-state coherent dynamics. (2 weeks)

Unit #2: Time varying potentials. Sudden vs adiabatic change. (1.5 weeks)

Unit #3: Density matrices; mixed and pure quantum states; property computation; quantum Liouville equation. (1.5 week)

Unit #4: Landau-Zener transitions and non-adiabatic dynamics, correlation functions. Ehrenfest dynamics, surface hopping, correlation functions. (Mr. Yuly, 1 week)

Unit #5: Time-dependent perturbation theory; Fermi's golden rule; driven electronic transitions; rotating wave approximation; field driven population transfer (coherent control, 2D spectroscopy). (1.5 weeks)

Unit #6: Introduction to 2D spectroscopy and system-bath interactions. (Prof. Zhang, 1.5 weeks)

Unit #7: Introduction to electron transfer (Franck-Condon factors, superexchange, Green's functions) (Mr. Valdiviezo, 1 weeks).

We will do focused readings from several textbooks and will use our developing text/guidebook to QD that aims at numerical solutions of model problems.

Learning objectives: Listed below are the broader learning objective for the semester. Specific learning objectives will be distributed with each individual unit (posted on Sakai). Given a summary of the key ideas for each unit (the "quick start guide"), students will learn to navigate the selected readings to understand the foundations and origins for each of the key ideas.

- Student will be able to translate from key ideas and foundational material to formulate solutions to chemically oriented problems in quantum dynamics.
- Students will develop the skills needed to use Python computation in Jypyter notebooks to solve problems in quantum dynamics and to communicate and interpret these solutions.
- Students will develop team skills to address complex problems in an open, collaborative environment.
- Students will synthesize their understanding of fundamental and applied aspects of quantum dynamics, their skills of communication using computation, and their team skills to create new "Chapters" of our developing text/workbook for use by future classes.