CHM1443F: Open Quantum Systems, Fall 2021

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Classes: Tue. 2-4 pm
Office Hours: Mon. 2-3 - or email me to set an alternative time.

Prerequisite: Graduate Quantum Mechanics CHM1478 (or its equivalents)
Learning Outcomes: Knowledge of central models, methods and applications in the area of open quantum systems; learning about quantum dissipation, electron and energy transfer processes in molecules and quantum devices; familiarity with computer simulations of time evolution in quantum mechanics; communication of scientific ideas and results; basic scientific programming

Marking Scheme
4-5 HW sets = 15-20% each. (penalty: 3 points/20 per day are taken for late submission)
Depending on class size: term paper or class presentation = 10%

Assignments
Submit on Quercus or in-person
Assignments will require you to perform simple simulations (recommended with MATLAB or Python).
UofT students can use Matlab Online / download and install MATLAB to their personally-owned machines **free of charge**. MATLAB (You do not need to install Matlab— Matlab Online is perfectly suitable)

Assignments	From	Due date	weight/100
set 1	Sep 14	Oct 05	20
set 2	Oct 05	Oct 19	20
set 3	Oct 19	Nov 09	20
set 4	Nov 09	Nov 23	15
set 5	Nov 23	Dec. 07	15
Term paper/class presentation (last classes)	Nov 30	Dec. 07	10

These are tentative dates, to be modified according to teaching pace. Please follow announcements in class and on the portal.

Academic Integrity
Please click, read and act with honesty: Academic Integrity at U of T and Code of behaviour of academic matters

Offenses include (but are not limited to): Using ideas of another person without acknowledgment; Submitting your work in more than one course without the approval of the instructor; Obtaining or providing unauthorized assistance on any assignment. Misconduct will be reported to the Associate Chair, Undergraduate/Graduate Studies

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Textbooks (No need to purchase):

- The Theory of Open Quantum Systems - H.-P. Breuer and F. Petruccione
- Chemical Dynamics is Condensed phases- A. Nitzan
- Nonequilibrium Statistical Mechanics- R. Zwanzig
- Statistical Mechanics: Theory and Molecular Simulation - Mark E. Tuckerman
- Quantum Dynamics: Application in Biological and Materials Systems - Eric R. Bittner

Syllabus:

1. Introduction to quantum relaxation processes:
   (i) Decay into a quasi-continuum (week 1-2)
   (ii) Relaxation of a quantum harmonic oscillator (week 3)
   (Nitzan, Sec. 9)

2. Density Operators and quantum master equations
   (i) Introduction to density matrix (week 4)
   (ii) Nakajima-Zwanzig equation and the Redfield equation (week 4-5)
   (iii) Examples: damped Harmonic oscillator, spin-boson model (week 6-7)
   (iv) Applications: Marcus theory for electron transfer, exciton dynamics (week 7)

   (Nitzan, Sec. 10, Breuer-Petruccione)

3. Pure decoherence and control schemes (week 8-9)
   (Breuer-Petruccione)

4. Classical and quantum Langevin equation
   Applications: Kramer's crossing rate, vibrational relaxation (week 10)

   (Zwanzig, Tuckerman)

5. Numerical solutions of the time dependent Schrödinger equation
   (i) Split operator methods (week 11)
   (ii) Feynman path integrals (week 12)

   (Tuckerman Chapter 12)

Announcements
Home assignments, solutions, and other important announcements will be posted on the CHM1443 website on Quercus. Please regularly check postings on Quercus.