CHM1443F: Open Quantum Systems, Fall 2021

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Please use your UofT email

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)

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