CHEM 501: Graduate course on Modern Applications of Quantum Mechanics in Science and Technology

Course outline

Roman Krems - rkrems@chem.ubc.ca; tel: (604) 827 3151; Office: D330

24 classes beginning on Wednesday, Sept 6, and ending on Wednesday, Dec 6, 2023

Classes: Monday and Wednesday at 1 pm – 2.30 pm, Room D317 (Chemistry building)

Midterm exam: Wednesday, **8 November 2023**, 1 pm, Room D317

Final paper: The final paper will be due by **Dec 20, 2023**.

Presentations: Most classes will include a 15-minute explanation of a particular topic by a student.

Problem sets: The homework problem sets will be marked and graded.

Grading: The final grade = homework problem sets (25 %), midterm exam (25 %), presentations (10 %), final paper (40 %).

The goals of the course are to:

- illustrate the beauty of quantum mechanics;
- review the most important concepts of quantum mechanics used in contemporary research;
- teach the students to think "quantum mechanically";
- discuss modern applications of quantum mechanics in science and technology';

Ultimate goal: at the end of the course, you should be able to describe how to predict the outcome of an experimental measurement for any given quantum system.

The final paper (due December 20, 2023) will be no more than five pages in single-column article format. The final paper will propose a quantum experiment to solve a research problem. "Experiment" means the work must involve a quantum measurement. The proposal must have the following sections: Introduction (to describe the problem to be solved); Motivation (to describe why the problem is interesting); Project Details (to describe the details of how the work would be performed); Expected outcomes (to describe the expected outcomes); and Quantumness (to describe why quantum mechanics is essential for this work).

Homework: There will be four homework problem sets developed to help students understand how quantum mechanics works. The problem sets will be marked and graded. You can use ChatGPT to help you understand how to answer the homework questions. However, all homework solutions must be hand-written and demonstrate your own understanding of the problems.

COURSE OUTLINE

Each class will thoroughly discuss the questions from the list below. The midterm examination will test the understanding of these questions.

Questions to be addressed in the course.

Week 1 (Sept 6):

1. Why does the time-dependent Schrödinger equation have this particular form

$$i\hbar\frac{\partial\psi}{\partial t} = \hat{H}\psi,$$

why is the momentum operator

$$\hat{p} = -i\hbar\frac{\partial}{\partial x}$$

and how to write the specific form of $\hat{H}$ for any given quantum system?

2. How do wavelike properties of electrons ensure that they do not collapse to the nucleus in an atom? (i.e. why is the atom stable?)

3. What is "waving" in the wave function and how does a measurement affect a quantum system?

4. What would atoms and molecules look like if the mass of the electron were twice its mass?

Week 2 (Sept 11 and 13):

5. When is an electron a classical particle and when is it quantum?

6. What is the relationship between quantum mechanics and classical mechanics?

7. How can the Ehrenfest theorem be used to establish the classical behaviour of a quantum particle?

Week 3 (Sept 18 and 20):

Student presentation 1: physical realization of qubits with trapped ions

Student presentation 2: physical realization of qubits with superconducting qubits

5. How can a quantum mechanical problem be formulated as an eigenvalue problem?

6. Why is quantum mechanics difficult or why do we need quantum computers?

7. Given the state of a quantum system at zero time, how can we predict the future behaviour of the system?

8. How to describe a qubit state by a vector on a Bloch sphere?

9. How to depict Rabi oscillations by the rotation of a vector on a Bloch sphere?

Week 4 (Sept 25 and 27):

Student presentation 3: spin echo

Student presentation 4: qubit entanglement - Bell's inequalities

10. What happens to a quantum system when it is exposed to classical electromagnetic field?
11. How to represent photons quantum mechanically?
12. How to represent the Hamiltonian for a many-body quantum system in second quantization?

Week 5 (Oct 4):

Student presentation 5: Coherent states

Student presentation 6: Density matrix description of coherent superpositions and statistical mixtures

13. What are dephasing and decoherence?
14. What is a quantum computer?
15. How does coupling to an environment change the quantum evolution or why is the world classical, or is it?

Week 6 (Oct 11 and 12):

Student presentation 7: Dicke superradiance

Student presentation 8: NV centres in diamonds as censors of magnetic fields

16. How to describe a collision of two atoms quantum mechanically?
17. How to describe a collision of an atom and a molecule quantum mechanically?
28. What is the scattering S-matrix and how to compute it?

Week 7 (Oct 16 and 18):

Student presentation 9: Measurement-based quantum computing

Student presentation 10: Trapped atoms as quantum pressure sensors

19. What is the Hubbard model and why is it important?
20. What is the difference between a quantum simulator and a quantum computer?

Week 8 (Oct 23 and 25):

Student presentation 11: Simulation of the Hubbard model with trapped atoms

Student presentation 12: Do birds use quantum mechanics for navigation?

21. What is the difference between the Frenkel and Wannier excitons?

22. What happens when excitons are coupled to phonons? What are polarons?

Week 9 (Oct 30 and Nov 1):

Student presentation 13: Does quantum mechanics play a role in photosynthesis?

Student presentation 14: Is our brain quantum?

23. What happens to electrons and atomic nuclei when molecules absorb or emit electromagnetic radiation?

24. What determines the spectroscopy selection rules?

25. Why do electrons have spin and why is it $s = 1/2$?

26. What would the atoms and molecules be like, if the electrons were bosons?

Week 10 (Nov 6 and 8):

Midterm exam: Nov 8

27. What are quantum gates and quantum circuits?

28. How does the IBM quantum computer work?

Week 11 (Nov 20 and 22):

Student presentation 15: How does the IBM computer entangle qubits?

Student presentation 16: How does the trapped ion quantum computer entangle qubits?

29. How to represent a Hamiltonian by an expansion in Pauli matrices?

30. What is the variational quantum eigensolver?

Week 12 (Nov 27 and 29):

Student presentation 17: How to solve a quantum chemistry problem on a quantum computer?

Student presentation 18: D-wave quantum annealer

31. What is machine learning?

32. How can machine learning be useful for chemistry?

Week 13 (Dec 4 and 6):

Student presentation 19: Computational complexity classes (P, NP, BQP)

Student presentation 20: Examples of problems that could benefit from quantum computing

33. What is quantum machine learning and how does it work?

34. Does quantum machine learning have a quantum advantage?

The following is background knowledge that you will acquire through self-study. If you need to review the topics mentioned in the table below, I recommend the following resources, or ChatGPT.

- "Introduction to Quantum Mechanics" by David J. Griffiths (second edition).
- "Introductory Quantum Mechanics" by Richard L. Liboff (fourth edition)

Please work through the material from the indicated pages of the Griffiths (G) and Liboff (L) books by the indicated date. The homework sets will test your understanding of this material.

Date	Topics	Textbook pages
Week 1	The Schrödinger equation, The statistical interpretation of Ψ, Normalization of Ψ, Coordinate and momentum representations, Fourier transforms, The Uncertainty Principle	G: All of Chapter 1, pages 1 - 24; L: All of Chapter 3, pages 68 - 89
Week 2	Stationary States, Particle in a box, Time evolution of wavepackets	G: Pages 25-40 of Chapter 2; L: Pages 152-170 of Chapter 6
Week 2	The energy-time uncertainty principle, Time derivative in quantum mechanics	G: Pages 114 - 124 of Chapter 3
Week 3	Hilbert Space, Dirac Notation	G: Pages 93 - 106 of Chapter 3
Week 3	Hilbert Space, Hermitian Operators, Eigenstates of Hermitian Operators	L: All of Chapter 4, Pages 90 -114
Week 3	Representing operators by matrices, Unitary transformations	L: Pages 480 - 504 of Chapter 11
Week 3	Time-independent Perturbation Theory	G: Pages 249 - 270 of Chapter 6 L: Pages 681 - 699 of Chapter 13
Week 3	Time-dependent Perturbation Theory	G: Pages 340 - 348 of Chapter 9 L: Pages 709 - 738 of Chapter 13
Week 4	The Harmonic Oscillator, The algebraic solution of the problem using the raising and lowering operators	G: Pages 40-67 of Chapter 2
Week 4	The Harmonic Oscillator, Correspondence Principle	L: Pages 202-207 of Chapter 7
Week 5	Hilbert Space, Hermitian Operators, Eigenstates of Hermitian Operators.	G: Pages 93 - 106 of Chapter 3; L: Pages 480 - 504 of Chapter 11
Week 6	Particle interacting with a delta-function potential (both barrier and well)	G: Pages 68 - 76 of Chapter 2; L: Pages 222-243 of Chapter 7
Week 6	Scattering by a delta-function potential (both barrier and well)	G: Pages 68 - 76 of Chapter 2; L: Pages 222-243 of Chapter 7
Week 9	Schrödinger equation in spherical polar coordinates, The Hydrogen atom	G: Pages 131 - 160 of Chapter 4
Week 9	Schrödinger equation in spherical polar coordinates, The Hydrogen atom	G: Pages 131 - 160 of Chapter 4
Week 9	Angular momentum in Quantum Mechanics	G: Pages 160 - 170 of Chapter 4 L: Pages 349 - 403 of Chapter 9
Week 9	Addition of Angular Momenta, Clebsch-Gordan Coefficients	G: Pages 184 - 189 of Chapter 4 L: Pages 349 - 403 of Chapter 9
Week 9	Electronic terms of Multi-electron atoms	G: Pages 210 - 218 of Chapter 5
Week 9	Emission and Absorption of Radiation	G: Pages 348 - 359 of Chapter 9
Week 9	Spectroscopy selection rules	G: Pages 359 - 363 of Chapter 9