C561: Atomic and Molecular Quantum Theory

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Instructor Officer hrs: Monday 1:30-3PM, Thursday 2:30-3:30PM (Chemistry C202B)

AI: Sowmya Ghosh. Office hours: Tuesday afternoon

The course will be conducted through detailed handouts. These notes are available at: http://www.indiana.edu/%7Essiweb/C561/C561.html **.**

You are responsible for downloading these notes before you come to class. Always check if an updated version is available.

In addition the following reference books are useful and are on reserve in the chemistry library.

- Modern Quantum Mechanics by J. J. Sakurai
- Elements of Quantum Mechanics by Michael D. Fayer
- Quantum Chemistry by Ira Levine
- Quantum Mechanics by Cohen-Tannoudji

Grading Policy:

1. Homeworks: 20 points. Homeworks are an important portion of this class and you will have homeworks *every week*.
   Homeworks are in the notes. You should read the notes carefully to make sure you do notmiss the homeworks. You are responsible for this. Homeworks are due every week, on Wednessdays.
2. One mid-term exam: 40 points
3. Final exam (cumulative): 40 points

Course outline:

The course website: http://www.indiana.edu/%7Essiweb/C561/C561.html serves as a detailed outline that is constantly updated. This document is not updated as often but does provide an overview of items that were covered in previous years.

Part I: Fundamental concepts

1. Course Outline
2. Handout: Linear algebra

Experimental considerations that provide a rationalization for the postulates of quantum mechanics.

3. The Stern-Gerlach Experiments To test the Stern-Gerlach experiments, download this nifty java applet. It will allow you to run the Stern-Gerlach experiments on your computer and understand it better. (You will need to have Java installed and enabled for this to run from the browser.) Click on the help menu to customize experiments.
4. The Stern-Gerlach experiments explained using plane polarized light and circularly polarized light
5. A brief summary of Stern-Gerlach experiments
6. de Broglie's Wave particle duality

Formal considerations that rationalize the Stern-Gerlach experiments and eventually lead us to the postulates of quantum mechanics.

7. Representation theory, Dirac notations, Hilbert space
8. Introduction to operators, Discrete and continuous representations, Coordinate and momentum representation, the quantum-mechanical Wavefunction
   The following additional material is related to what we have learned thus far. Hence please go over these yourself. We will cover it later in class, quickly. If you have trouble see me. You are responsible for the homework problems in these sections.
   Simultaneous additional reading: Important Summary of Dirac notation
   Simultaneous additional reading: Theory of Operators: I
   Simultaneous additional reading: Pauli Spin matrices
   Simultaneous additional reading: Change of basis
   Simultaneous additional reading: The Concept of Measurement in quantum mechanics
9. Postulates of Quantum mechanics
   Homework: Justify the stated postulates through your knowledge of the Stern-Gerlach experiments.

The statement on "uncertainty" is really a result of the vector spaces idea that we have discussed above.

10. Simultaneous observables, Commutation relations, expectation values
11. Uncertainty Principle and Coherent states

The Schrodinger Equation and associated properties.

12. The Time dependent Schrodinger Equation
    Simultaneous additional reading: Solving the time-dependent Schrodinger Equation.
    Simultaneous additional reading: The Classical limit and the WKB theory
    Simultaneous additional reading: Probability Current and the continuity equation.
    Simultaneous additional reading: Dirac quantization, The Schrodinger picture and the Heisenberg

Picture, Heisenberg's equation of motion (The Heisenberg's equation of motion is analogous to the time-dependent Schrodinger Equation, but as we see here provides connections to classical mechanics as well)
At this point you may wish to read a little about the history of quantum mechanics . The link above oulines some of the struggles between Schrodinger and Heisenberg in arriving at a unifying picture of quantum mechanics. It is Dirac's path that we have chosen in this class, which does unify the two pictures. In addition, through the set of readings provided here, you may see that the connections to classical mechanics can be quite exciting.

13. The Time independent Schrodinger Equation.
    Simultaneous additional reading: Theory of Operators: II. Hermitian operators and their properties.

Part II: Analytically solvable model problems for free-particle

14. Particle-in-a-box
    Simultaneous additional reading: The concept of Resonance in delocalized Pi electron systems from particle-in-a-box
    Simultaneous additional reading: Quantum Confinement: Applications to quantum dots, Fermi gas, Thomas-Fermi theory (and functional)
15. Other one-dimensional problems: scattering off a step function, scattering off a square potential barrier, reflection and transmission coefficients, scattering cross sections in 1D, relation to thermal rate constants
16. Time-evolution of a state that is written as a linear combination of eigenstates. Two-state problem.

Part III: Concepts behind solutions to atomic and molecular problems

17. Harmonic Oscillator
18. Simultaneous additional reading: Harmonic Oscillator solution (Hermite functions)
19. Harmonic oscillator revisited: Dirac's approach and introduction to Second Quantization
20. Theory of Angular Momentum I: Ladder operators
    Simultaneous additional reading: Spherical Harmonics: Transforming the angular momentum problem in radial coordinates
    Simultaneous additional reading: Introduction to Electron nuclear systems
    Simultaneous additional reading: Permutation symmetry of electrons: Fermionic and Bosonic systems, Pauli's exclusion principle, Bose-Einstein condensation
21. Theory of Angular Momentum II: Clebsch-Gordon coefficients
    Simultaneous additional reading: When would you need Angular momentum addition and Clebsch Gordon coefficients?

22. Hydrogen Atom
    Simultaneous additional reading: Generating functions
    Simultaneous additional reading: Orthogonal Polynomials
23. Variational Principle
24. Independent Particles, Hartree product, Slater determinants
25. Group Theory