C561: Atomic and Molecular Quantum Theory

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Office Hours Monday 1:30-3PM, Thursday
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The course will be conducted through detailed handouts. These notes are available on the web:
http://www.indiana.edu/%7Essiweb/C561/C561.html

You are responsible for dowloading 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 kept 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 not miss 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

A detailed course outline is the course website itself. The following list is only suggestive and is not updated as frequently as the course website.

Part I: Fundamental concepts:
Experimental considerations that provide a rationalization for the postulates of quantum mechanics.

1. Reasons why we learn quantum mechanics: Predicting chemical properties, reactivity, spectroscopy using theory
2. The need for a new physics: Illustrations using the Stern-Gerlach experiments.
   The Stern-Gerlach experiments are a sequence of experiments that expose the pitfalls of the old classical physics. The new laws of modern physics, the quantum theory, can be seen as a direct consequence of these experiments. This discussion will directly lead us into important concepts including:
   (a) The postulates of quantum mechanics: In fact we will see that the postulates of QM can be nicely understoond from our treatment of the SG experiments. In the process we will also learn about the three items below.
   (b) Similarity of spin states to plane and circularly polarized light
   (c) Spin Quantization
   (d) The requirement of a wave-particle duality

   This will allow us to embark into a full fledged treatment of quantum theory. An understanding of linear algebra and vector spaces is, however, essential to proceed further and you are asked to review this using the provided handouts.
3. de Broglie's wave-particle duality
   Formal considerations that rationalize the Stern-Gerlach experiments and eventually lead us to the postulates of quantum mechanics.
4. Basic ideas of representation theory
   (a) Discrete representations: Generalization from simple three dimensional treatment
   (b) Dirac Algebra (Bra-Ket algebra)
   (c) Continuous representations
   (d) Operators, eigenvectors and eigenvalues
   (e) Position and Momentum representations
   (f) The Wavefunction
5. Heisenberg's Uncertainty principle: The statement on "uncertainty" as we will see is really a result of the vector spaces idea that we have discussed above. The result of our treatment of the SG experiments.

   (a) Simultaneous observables, Commutation relations
   (b) Coherent states

The Schrodinger Equation and associated properties.

6. The time-dependent Schrödinger equation
7. The time-independent Schrödinger equation
8. The theory of Operator
   (a) Hermitian operators
   (b) commutators

Part II: Analytically solvable model problems for free-particle:

9. Particle in a box: An approximation to unsaturated hydrocarbons
   (a) One dimensional simple box
   (b) Other problems in 1D: Introduction to quantum tunneling and over the barrier reflection
   (c) Brief introduction to scattering, and calculating thermal rate constants
10. Time evolution, two-state problem, Rabi frequencies.

Part III: Concepts behind solutions to atomic and molecular problems

11. The Harmonic Oscillator
   (a) Ladder operators
   (b) Second Quantization
12. Angular momentum
13. Hydrogen atom
14. Introduction to Electron-nuclear systems
   (a) The Born Oppenheimer and adiabatic approximation
   (b) The full Non-adiabatic case
   (c) Born Oppenheimer dynamics
15. Variational principle
16. Permutation symmetry of electrons:
   (a) Independent particle and the Hartree product
   (b) Slater determinants
   (c) Introduction to Hartree-Fock theory
17. Group theory
   (a) Point groups

   (b) Group representation theory and character tables
   (c) Projection operators
   (d) Symmetry adapted linear combinations

18. Perturbation theory

