CHM 421: Physical Chemistry 1
Quantum Mechanics

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Course description: An introduction to the principles of Quantum Mechanics and applications to simple systems

Course Details

1. **Review of Classical Mechanics:** Particle, waves and fields, Newton's laws of motion, Lagrangian and Hamiltonian formulations. (3 lectures)
2. **Historical Perspective:** Origin of new physics, Black body radiation, electron diffraction, photoelectric effect, wave-particle duality, uncertainty principle, wave functions and interpretation (5 lectures)
3. **Framework of Quantum Mechanics:** Operators, Expectation values, commutation relations, fermions and bosons, Hermitian operators, eigenvalues and eigenvectors, matrix representations, bra-ket notations, position representation (6 lectures)
4. **Schrödinger Equation:** Time dependent Schrödinger equation, stationary states, Time independent Schrödinger equation, Quantization (2 lectures)
5. **Exactly Solvable Model Systems:** Particle in a container, Free particle, momentum representation, plane waves, tunneling, 1-dimensional simple harmonic oscillator, classical and quantum oscillator, vibrational energy, anharmonicity, 1-D and 3-D rigid rotor, angular momentum, Hydrogen atom, Pauli's exclusion principle, electron spin, 2nd quantization (14 lectures)
6. **Beyond Exactly Solvable Models:** H_2^+,many electron wavefunctions, He, H_2, Slater determinants, variational theories, perturbation theories, addition of angular momentum, term symbols (8 lectures)
7. **Dynamics:** Schrödinger and Heisenberg formulations, Feynmann Path Integrals (3 lectures - if time permits)

Books:

There is no prescribed book for this course. I prefer to make my notes after reading different books. There are many excellent books in Quantum Mechanics and you will be well-served by reading one or more of them. However, it is good to be a little cautious while going through any book. There are many subtleties in the subject and this can often lead to incorrect descriptions even in books by well known authors. In addition to the books, there are numerous online resources in Quantum Mechanics. Once again, beware of possible errors. I have listed some books and references which you may find useful, but there are many others too.

1. I.N. Levine, *Quantum Chemistry*
2. Claude E. Cohen-Tannoudji, Bernard Liu and Franck Laloë, *Quantum Mechanics Volume I*
3. John P. Lowe and Kirk A. Peterson, *Quantum Chemistry*
4. P.W. Atkins *Molecular Quantum Mechanics*
5. Tom Engel and Philip Reid, *Physical Chemistry*
6. P.W. Atkins and Julio de Paula *Physical Chemistry*
7. Michael D. Fayer *Elements of Quantum Mechanics*
8. Herbert Goldstein *Classical Mechanics*
9. Linus Pauling and E. Bright Wilson, *Introduction to Quantum Mechancs*
10. J.J. Sakurai, *Modern Quantum Mechanics*
11. L.D. Landau and E.M. Lifshitz, *Course of Theoretical Physics Vol 3. Quantum Mechanics (Non-relativistic theory)*
12. R. McWeeny, *Quantum Mechanics: Principles and Formalism*

Internet Resources

1. http://hyperphysics.phy-astr.gsu.edu/hbase/hph.html This website is hosted by the department of Physics and Astronomy at Georgia State University. The chart gives a great overview of Quantum Mechanics. Individual links on the chart show more details of the phenomena. It is easy to read and allows you to get a broad overview without going into too many details.
2. http://ocw.mit.edu/OcwWeb/Chemistry/5-73Fall-2005/CourseHome/index.htm : This is part of MIT open course ware. The notes here are excellent and the orientation is very modern. It does not track the historical development much, and the arrangement of content is different from usual books.
3. http://arxiv.org/abs/quant-ph/0605180 Lecture Notes in Quantum Physics by Doren Cohen. This set of notes puts Quantum Mechanics in a beautiful mathematical framework. The emphasis here is not on solving simple model systems, but rather to examine some of the mathematical features that lead to quantum mechanics. It requires a good background in classical mechanics and some advanced abstract algebra. You can try to read the first section of these notes.

Grading System

1. Homework Assignments: 25 %
   These will consist of 5 assignments. You have one week to complete the assignments. The assignments will be given in class and will be due in class a week later. You are encouraged to speak to each other and work together on assignments, but each person has to submit their own assignment in their own handwriting. Late assignments will be penalized at the rate of 20% per day.

2. Mid Semester 1 : 15 %
   This will be an in-class exam lasting 1 hour. The exam is open book/notes. However, you are not allowed to share study materials or calculators.

3. Mid Semester 2 : 15 %
   This will be a week long take-home exam. You are not allowed to speak to any one about the exam or copy or take any help from anyone.

4. Final Exam : 45 %
   This will be an in-class exam lasting 3 hours. The exam is open book/notes. Again, you are not allowed to share study materials or calculators.

Letter Grades: Letter grades will be awarded based on the total marks out of 100. The grades will be based on the class average(A) and the standard deviation (σ). Passing marks for the course will not be higher than $A - 3\sigma$.

Warnings: Any misdemeanor during the exams will immediately result in the student obtaining zero marks for the exam. Further misdemeanor will result in an F grade for the student.

My Objectives of this course:

- Make you familiar with the machinery of quantum mechanics
- Understand quantum mechanics better myself
- Inspire you enough to read one of the last 3 books listed