Chem 532

Advanced Physical Chemistry II – Quantum Mechanics

Fall 2015

Syllabus

Instructor: Dr. David Y. Lee

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Office Hours: Stop by anytime or by appointment.

Prerequisite: Chem 332 or equivalent

Course Materials & Resources:

For this particular graduate level QM course for chemists, the recommended textbook is Fayer[1]. This book was chosen because it (**1**) is concise and readable; (**2**) uses "modern" *Dirac* Bra–Ket notations; and (**3**) was born from the author's lecture notes teaching the exact same graduate course at Stanford. Another commonly adopted textbook in similar graduate courses is Shankar[2]. Bohm[3] is a much less expensive, more comprehensive but still readable textbook. It, however, was written in "the old language", *i.e.* integrals, instead of *Dirac* Bra–Ket notations. If you would prefer an reference, high level and non-readable (at least to me in terms of how the authors organized the topics) style textbook, Cohen-Tannoudji (an Nobel laureate) *et al.*[4] will not disappoint you. Atkins and Friedman[5] is also a good choice especially if you are/will be taking the graduate spectroscopy course. There is a copy of Cohen-Tannoudji *et al.*[4] and an older edition of Atkins and Friedman[5] reserved at the Owen Science & Engineering Library. Fayer also published a descriptive QM book[6] for non-scientific readers. I strongly suggest that you obtain a personal copy of Bohm[3] in addition to the book of your choice. For those of you needing extra help in mathematics, I would recommend Steiner[7] over the reference-style McQuarrie[8].

Evaluation:

Problem Sets: 55%

Mid-Term: 15%

Final: 30%

There will be ∼7–8 problem sets graded for this course. Your highest PS score *after and not including* PS#0 will be excluded from your total PS grade and counted as your mid-term grade (PS#0 is review of undergraduate QM and math + some Classical Mechanics). In the end of the course, there will be a cumulative final exam (format and date to be determined).

Grading Scale:

80–100%	**A**
60–79%	**B**
≤59%	**C**

Course Outline:

1. **Prelude: Fast Introduction/Review of Matrix Algebra**
   - The 2D Rotation Matrix
   - Inverse and Orthogonal Transformation
   - Eigenvalues and Eigenvectors; Matrix Diagonalization
   - Hermitian Matrices
2. **Absolute Size & The (Quantum) Superposition Principle**
3. **Classical Mechanics**
   - $\boldsymbol{F} = m\ \boldsymbol{a}$
   - Fourier Analysis
   - Lagrangian Formulation
   - Hamiltonian Formulation
4. **Wave (State) Equations for Matter**
   - Bohr's Atomic Model
   - De Broglie Waves
   - The Schrödinger Equation
   - The Hydrogen Atom
   - Pauli Exclusion Principle and the Spin Quantum Number
   - Shell & Subshells; Removal of Degeneracy
5. **Hilbert Space**
   - The Correspondence Principle and the Copenhagen Interpretation
   - Average Values and the Ehrenfest Theorem
   - Hermitian Operators and Orthonormal Eigenfunctions
   - Discrete and Continuous Spectra of Eigenvalues
   - The *Dirac* Bras and Kets
   - Wavepackets and Fourier Transform between Position and Momentum Spaces
   - The Uncertainty Principle
6. **Boundary Conditions & Quantization of Energy**
   - Curvature, Sign and Acceptability of the Wavefunctions
   - Penetration into Non-Classical Regions
   - Particle in a Box
   - Harmonic Oscillator

7. **Angular Momentum in QM**
    - Angular Momentum in CM
    - Angular Momentum Operators, Matrix Elements and Eigenfunctions
    - Addition of Angular Momentum and Clebsch-Gordan Series
    - Spin
8. **Approximation Methods**
    - The Variation Principle
    - Perturbation Theory
    - ∗ WKB Approximation
9. **Fundamental Theory of Chemical Bonding**
    - H_2^+
    - H_2
    - Hybridization
    - ∗ Electronic States of Diatomic Molecules
10. ∗ **Multi-Electron Problems**
    - Slater Determinants
    - Hartree-Fock Equation and the Self-Consistent Field (SCF) Method
    - Restricted and Unrestricted SCF for Open Shells
    - Configuration Interactions

∗ If we have time

Course Rules & Academic Integrity
The problem sets are designed to motivate you to *read the accredited books* and to *contemplate the subjects*, not as means to simply grade you. For each problem set, you are welcome to use computational programs such as *Mathematica* to work on each problem (except for those problems marked with ✍) and to simply submit the print-out results. However, you *MUST* develop and type your own code. Discussion among members of this class is also **encouraged**; but if a particular question is marked with ☹, you are *NOT* allowed to discuss it with anyone and *MUST* work on it by yourself. Consultation to **the internet** and **last year's answer keys** is also prohibited for every work you turn in; if you find a website containing necessary information for your work, please contact me before using it.

WSU Academic Integrity Statement

"As an institution of higher education, Washington State University is committed to principles of truth and academic honesty. All members of the University community share the responsibility for maintaining and supporting these principles. When a student enrolls in Washington State University, the student assumes an obligation to pursue academic endeavors in a manner consistent with the standards of academic integrity adopted by the University. To maintain the academic integrity of the community, the University cannot tolerate acts of academic dishonesty including any forms of cheating, plagiarism, or fabrication. Washington State University reserves the right and the power to discipline or to exclude students who engage in academic dishonesty."

Students found responsible for academic integrity violations may receive an **F** on the particular assignment or exam, as well as an **F** for the course. Repeated and/or serious offenses may result in referral to the conduct board and **expulsion from WSU**. For graduate students, academic integrity violations may also result in the loss of teaching and/or research assistantships.

Students with Disabilities

Reasonable accommodations are available for students with a documented disability. If you have a disability and need accommodations to fully participate in this class, please either visit or call the Access Center (Washington Building 217; 509-335-3417) to schedule an appointment with an Access Advisor. All accommodations MUST be approved through the Access Center.

Bibliography

[1] M. D. Fayer. *Elements of Quantum Mechanics*. Oxford University Press, .

[2] R. Shankar. *Principles of Quantum Mechanics*. Plenum Press.

[3] D. Bohm. *Quantum Theory*. Dover Publications.

[4] C. Cohen-Tannoudji *et al.* *Quantum Mechanics*. Wiley.

[5] P. W. Atkins and R. S. Friedman. *Molecular Quantum Mechanics*. Oxford University Press.

[6] M. D. Fayer. *Absolutely Small: How Quantum Theory Explains Our Everyday World*. AMACOM, .

[7] E. Steiner. *The Chemistry Maths Book*. Oxford University Press.

[8] D. A. McQuarrie. *Mathematical Methods for Scientists and Engineers*. University Science Books.