

Chemistry 5210
Advanced Physical Chemistry I: Quantum Mechanics

Fall 2016
Ian Harrison

Nature of the Course

This course provides an introduction to quantum mechanics for scientists and engineers interested in the properties and phenomena of atomic, molecular, and nanoscale matter. The foundational ideas of quantum mechanics are introduced and tools for exact and approximate solutions of the Schrodinger Equation are developed. Model systems, such as particle in a box, harmonic oscillator, hydrogen atom, hydrogen ion and molecule, crystalline solids, as well as time-dependent phenomena, such as spectroscopy, tunneling, and scattering, are examined as time permits. The course aims to provide the elementary background and tools necessary to read and advance modern research requiring a microscopic understanding of matter.

Textbook

- 1) *Quantum Mechanics for Scientists and Engineers*, by D. A. B. Miller, Cambridge University Press, 2008. – broadly ranging text with useful appendices on background math and physics.

Possibly Useful Companion References

- 1) *Quantum Mechanics in Chemistry* by G. C. Schatz, and M. A. Ratner, Dover, Mineola, N.Y., 2002 – more advanced than the text, terser, focused on chemistry, and only ~\$15.
- 2) *Elements of Quantum Mechanics* by M. D. Fayer, Oxford University Press, New York, NY, 2001 – less advanced, terser, focused on chemistry, but with somewhat unusual notation.
- 3) *Introduction to Quantum Mechanics* by D. J. Griffiths, Pearson Prentice Hall, Upper Saddle River, NJ, 2005 – a viable, less encyclopedic, alternative to the text.

Resources

- 1) Reserve books in Chemistry Library, Rm. 259

Course Calendar

1) Course Meeting Times:

Monday, Wednesday & Fridays 10:00 am-10:50 pm. in Rm. 305 of the Chemistry Building.

2) Marking Scheme:

Problem Sets (4)	60% (Due Sept 14, Oct. 12, Nov. 7, Dec. 2)
Midterm	10% (Oct. 19)
Final Exam	30%

Professor Harrison's office is Rm. 154

labs are Rms. 150, 162, 204

secretary is Susie Marshall in Rm. 188

email: harrison@virginia.edu

Chemistry 5210

Reserve Books for Chemistry Library

- 1) *Quantum Mechanics for Scientists and Engineers*, by D. A. B. Miller, Cambridge University Press, 2008 – course text
- 2) *Quantum Mechanics in Chemistry* by G. C. Schatz, and M. A. Ratner, Dover, Mineola, N.Y., 2002 – more advanced than the text, terser, focused on chemistry, and only ~\$15.
- 3) *Elements of Quantum Mechanics* by M. D. Fayer, Oxford University Press, New York, NY, 2001 – less advanced, focused on chemistry, but with unusual notation.
- 4) *Introduction to Quantum Mechanics* by D. J. Griffiths, Pearson Prentice Hall, Upper Saddle River, NJ, 2005 – a viable, less encyclopedic, alternative to the text.
- 5) *Quantum Mechanics*, Vols 1 & 2, by C. Cohen-Tannoudji, B. Diu, and F. Laloe, Wiley, 1991 – elegant rather complete exposition by French authors, but expensive.
- 6) *Quantum Mechanics* by A. Messiah, Dover Publications, Mineola, NY, 2014 – reprint of an excellent older text in the elegant French style.
- 7) *Modern Quantum Mechanics* by J. J. Sakurai, and J. Napolitano, Addison-Wesley, 2011- more advanced physics oriented text.
- 8) *Principles of Quantum Mechanics* by R. Shankar, Springer US, 2011 – more advanced and encyclopedic physics text.
- 9) *The Principles of Quantum Mechanics* by P. A. M. Dirac, 4th ed. revised, Clarendon Press, Oxford, 1967. – update of the seminal 1928 quantum text.
- 10) *Quantum Mechanics: Non-Relativistic Theory* by L. D. Landau, and E. M. Lifshitz, Pergamon Press, Oxford, 1977 – Volume 3 of their course in theoretical physics.
- 11) *Introduction to Quantum Mechanics: A Time-Dependent Perspective* by D. J. Tannor, University Science Books, 2007.
- 12) *Electronic Structure: Basic Theory and Practical Methods* by R. M. Martin, Cambridge University Press, 2004.
- 13) *Modern Quantum Chemistry: Introduction to Advanced Electronic Structure Theory* by A. Szabo, and N. S. Ostlund, Dover Publications, Mineola, N.Y., 1996.