课程代码（Coursenumber）
Chemistry 7940 (794)

课程对象（Audience）
Primarily for Graduates

开课教师（Teacher）
Professor Ezra

学期（Semester）
Spring

课程描述（Description）
课程提纲（Syllabus）
1. Approximation methods in QM: WKB theory
• Motivation. Short-wavelength limit of Schr¨odinger equation.
• WKB approximation. Conditions for validity.
• Connection formulas.
• Applications: 1D bound states. 1D barrier penetration.
2. Density matrix
• Pure vs mixed states. Ensemble interpretation.
• Reduced density matrices.
• Correlation & entanglement.
• Equations of motion. Analogy with classical mechanics.
• Relaxation and decoherence.
3. Time-dependent phenomena
• Evolution operator. Propagators and Green’s functions.
• Three pictures: Schr¨odinger, Heisenberg, interaction.
• 2-level system. Rotating wave approximation. Bloch equations.
• Time-dependent perturbation theory. Harmonic perturbations. Resonant phenomena. Transitions
to a continuum. Fermi’s Golden rule.
• Sudden approximation.
• Adiabatic approximation. A geometric phase.
• Perturbation theory for the density operator. Linear response.
4. Path integral formulation of quantum mechanics
• Derivation of the sum-over-paths expression for the propagator.
• Semiclassical limit of the path integral.
5. Molecule-field interactions
• Maxwell’s equations, scalar and vector potentials, gauge transformations, free field, and all
that.
• Hamiltonian for charged particle in field.
• Perturbation in dipole approximation.
• A and B coefficients. Selection rules. Sum rules.
• Electric quadrupole and magnetic dipole transitions.
• High-order perturbation theory and multiphoton processes.
1 of 2
• Nonlinear spectroscopy.
• Electric properties of molecules. Polarizability.
• Magnetic properties of molecules. Magnetic susceptibility. Diamagnetism & paramagnetism.
• Quantizing the EM field. Photons. Spontaneous emission revisited.
6. Quantum mechanics of the continuum: Scattering theory
• Particle flux and scattering cross sections.
• Green’s functions and the scattering problem.
• Born approximation.
• Partial wave analysis of wavefunction for central scattering potential.
• Phase shifts and differential cross section.
7. Molecular electronic structure
• We are not addressing this topic, as the subject is being treated in detail by Professor Chan
in Chem 7980, Bonding in Molecules.
If we have time:
8. Molecular vibrations
• Born-Oppenheimer approximation.
• Rotation-vibration separability.
• Normal modes.
• Vibration-rotation transitions. Selection rules. Polarization.

课时信息（Totalhours）
16696 LEC 001 TR
03:00PM - 04:30PM
CLK 609
Hines,M (mah11

教参信息（Textbookinfo）
1 Physical Chemistry: A Molecular Approach by Donald A. McQuarrie and John D. Simon (Hardcover - July 1, 1997)
ISBN-13: 978-0935702996
2 Quantum Mechanics in Chemistry (Physical Chemistry Textbook Series) by Melvin H. Hanna (Paperback - Feb. 1981)
ISBN-13: 978-0805337051
3 Introduction to Quantum Mechanics with Applications to Chemistry by Linus Pauling and E. Bright Wilson Jr. (Paperback - Mar. 1, 1985)
ISBN-13: 978-0486648712
4 Inorganic Chemistry by James House and James E. House (Paperback - Aug. 8, 2008)
ISBN-13: 978-0123567864
世界各地拥有馆藏的图书馆（OCLC）:207
5 Computational Chemistry: Introduction to the Theory and Applications of Molecular and Quantum Mechanics by Errol Lewars (Paperback - June 1, 2010)
ISBN-13: 978-9048138616
世界各地拥有馆藏的图书馆（OCLC）:2
6 Compendium of Quantum Physics: Concepts, Experiments, History and Philosophy by Daniel Greenberger, Klaus Hentschel, and Friedel Weinert (Hardcover - Sept. 9, 2009)
ISBN-13: 978-3540706229
世界各地拥有馆藏的图书馆（OCLC）:169
7 Quantum Mechanics in Chemistry (Topics in Physical Chemistry) by Jack Simons and Jeff Nichols (Hardcover - Jan. 30, 1997)
ISBN-13: 978-0195082005
8 Quantum Mechanics in Chemistry by George C. Schatz and Mark A. Ratner (Paperback - Jan. 28, 2002)
ISBN-13: 978-0486420035
世界各地拥有馆藏的图书馆（OCLC）:77
9 Molecular Quantum Mechanics by Peter Atkins and Ronald Friedman (Paperback - Feb. 17, 2005)
ISBN-13: 978-0199274987
世界各地拥有馆藏的图书馆（OCLC）:170
10 Beyond Measure: Modern Physics, Philosophy, and the Meaning of Quantum Theory by Jim Baggott and Peter Atkins (Paperback - Jan. 1, 2004)
ISBN-13: 978-0198525363
世界各地拥有馆藏的图书馆（OCLC）:470
11 Chemical Modeling: From Atoms to Liquids by Alan Hinchliffe (Hardcover - Nov. 1, 1999)
ISBN-13: 978-0471999034