Chemistry 6491: Quantum Mechanics
List of Important Concepts

The following is a list of most of the important concepts covered in this course. It is not guaranteed to be 100% complete.

Unit I: Overview, Mathematical Introduction

1. The Schrödinger equation, time dependent and time independent.
2. Linear vector spaces
   (a) Definition of complex numbers, complex conjugate, and absolute value squared of complex numbers
   (b) Definition of a linear vector space
   (c) Definition of a basis set
   (d) Definition of linearly dependent / independent sets of vectors
   (e) Inner and outer products
   (f) Dirac (bra-ket) notation. Connection between kets and column vectors, and between bras and row vectors
   (g) Definition of a dual space
   (h) Definition and use of adjoints
   (i) Definition of an eigenvalue equation, eigenvalues, and eigenvectors
   (j) Matrix/vector operations: vector dot products, matrix-vector multiplication, matrix/matrix multiplication, how to find eigenvalues and eigenvectors of a matrix
3. Operators
   (a) Definition of an operator
   (b) Definitions of linear and anti-linear operators
   (c) Basic rules for operators; general non-commutativity of operators
   (d) Hermitian operators and their properties
   (e) Unitary operators and their properties
4. What is meant by a "change of basis." How to change from one basis to another
5. Diagonal form of a matrix; definition of a similarity transform and a unitary transform

6. How matrix diagonalization can "uncouple" classical problems, the classical propagator (how states evolve in time from a given initial state), and how this relates to quantum mechanics

7. Commutators

    (a) Definition of a commutator

    (b) Two operators commute if their commutator is zero

    (c) Basic rules of commutators

    (d) Using arbitrary functions to get the product rule right, as in $[x, \hat{p}_x]$

    (e) Campbell-Baker-Housdorff theorem

    (f) Simultaneous eigenvectors: what this means, connection to postulates and commutators

8. Infinite dimensional vector spaces (Hilbert spaces): Connection between Dirac notation and function notation, e.g., $\langle x|f\rangle = f(x)$, and Dirac delta functions

9. X space vs P space and converting between the two

10. **Postulates of quantum mechanics**

    (a) What are the postulates of quantum mechanics

    (b) What the postulates of quantum mechanics mean

    (c) Interpretation of $\Psi(x)$ and of $\Psi^*(x)\Psi(x)$, and how this connects to normalization

    (d) Only eigenvalues can be observed. How to determine what values are allowed in general, or in measurements of a given state Ψ, and the probability of each (including degeneracies)

    (e) Average value formula and uncertainty

    (f) Collapse of the wavefunction

11. Density matrices in quantum mechanics

12. Generalization from 1D to many dimensions

13. **General strategies for solving the Schrödinger equation, and time dependence**. How to get time-dependent solutions from time-independent solutions. How a wavefunction changes in time. The quantum propagator. Meaning of stationary states.

14. Particle in a box: the Hamiltonian and boundary conditions, how the boundary conditions lead to allowed solutions, the eigenvalues and eigenfunctions

15. Free particle: the Hamiltonian, eigenfunctions, eigenvalues, and how to do delta function normalization

16. Separability
    (a) Definition of separability, when a problem is separable, what the wavefunction and eigenvalues look like when a problem is separable
    (b) 3D particle in a box: how to solve

Unit II: Fundamentals

1. Ehrenfest's Theorem: What is says, what it means, how it helps relate quantum and classical mechanics
2. Harmonic oscillator: What the Hamiltonian is, Hooke's law, why harmonic oscillator is important in chemistry, how the wavefunction needing to go to zero at infinity is a kind of "boundary condition" that leads to quantization, what the eigenvalues are, what the eigenfunctions look like (including their even/odd character), how to work simple diatomic molecule harmonic oscillator problems (including working with the wavenumber unit of energy)
3. Second quantization: what is second quantization, what are raising and lowering operators, how do they work, how to solve harmonic oscillator in second quantization, how to get matrix elements using second quantized operators for harmonic oscillator
4. Heisenberg uncertainty relations: what the Heisenberg uncertainty relation says, how it is not just about position and momentum but about any pair of non-commuting operators, what it has to do with commutators
5. Spherical polar coordinates: how they are defined, what the kinetic energy operator looks like in spherical polar coordinates, the extra factors in the "volume element" required when integrating in spherical polar coordinates
6. Angular momentum: definition of the angular momentum operators, how those operators commute (or not), the rigid rotator problem and its eigenfunctions and eigenvalues, what spherical harmonics are and their properties, degeneracy of spherical harmonics, what ladder operators are in angular momentum and how they work, geometrical interpretation of quantum angular momentum (pictures of cones)
7. Properties of spherically symmetric problems, what a radial Schrödinger equation is
8. H atom: what is the Hamiltonian, fact that it is a spherically symmetric problem, how to solve the angular vs the radial parts, what the energies are, basics of what the wavefunctions look like and their properties (number of radial and angular nodes, their degeneracies, etc)