

高等物理化學二

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一. 內容

1. THE SCHRÖDINGER EQUATION

- 1.1 Quantum Chemistry
- 1.2 Historical Background of Quantum Mechanics
- 1.3 The Uncertainty Principle
- 1.4 The Time-Dependent Schrodinger Equation
- 1.5 The Time-Independent Schrodinger Equation
- 1.6 Probability
- 1.7 Complex Numbers
- 1.8 Units

2. THE PARTICLE IN A BOX

- 2.1 Differential Equations
- 2.2 Particle in a One-Dimensional Box
- 2.3 The Free Particle in One Dimension
- 2.4 Particle in a Rectangular Well
- 2.5 Tunneling

3. OPERATORS

- 3.1 Operator
- 3.2 Eigenfunctions and Eigenvalues
- 3.3 Operators and Quantum Mechanics
- 3.4 The Three-Dimensional Many-Particle Schrodinger Equation
- 3.5 The particle in a Three-Dimensional Box
- 3.6 Degeneracy
- 3.7 Average Values
- 3.8 Requirements for an acceptable Wave Function

4. THE HARMONIC OSCILLATOR

- 4.1 Power-Series Solution of Differential Equations
- 4.2 The One-Dimensional Harmonic Oscillator
- 4.3 Vibration of Molecules

5. ANGULAR MOMENTUM

- 5.1 Simultaneous Measurement of Several Properties

- 5.2 Vectors
- 5.3 Angular Momentum of a One-Particle System
- 5.4 The Ladder-Operator Method for Angular Momentum

6. THE HYDROGEN ATOM

- 6.1 The One-Particle Central-Force Problem
- 6.2 Noninteracting Particle and Separation of Variables
- 6.3 Reduction of the Two-Particle Problem to a One-Particle Problem
- 6.4 The Two-Particle Rigid Rotor
- 6.5 The Hydrogen Atom
- 6.6 The Bound-State Hydrogen-Atom Wave Function
- 6.7 Hydrogenlike Orbitals
- 6.8 The Zeeman Effect

7. THEOREMS OF QUANTUM MECHANICS

- 7.1 Introduction
- 7.2 Hermitian Operators
- 7.3 Expansion in Terms of Eigenfunctions
- 7.4 Eigenfunctions of Commuting Operators
- 7.5 Parity
- 7.6 Measurement and the Superposition of States
- 7.7 Position Eigenfunctions
- 7.8 The Postulates of Quantum Mechanics
- 7.9 Measurement and the Interpretation of Quantum Mechanics

8. THE VARIATION METHOD

- 8.1 The Variation Theorem
- 8.2 Extension of the Variation Method
- 8.5 Linear Variation Functions

9. PERTURBATION THEORY

- 9.1 Introduction
- 9.2 Nondegenerate Perturbation Theory
- 9.3 Perturbation Treatment of the Helium-Atom Ground State
- 9.5 Perturbation Theory for a Degenerate Energy Level
- 9.9 Time-Dependent Perturbation Theory
- 9.10 Interaction of Radiation and Matter

10. MOLECULAR SPECTROSCOPY

- 10.1 Transition Dipole Moment

- 10.2 Population Difference
- 10.3 Franck-Condon Principle
- 10.4 Franck-Condon factors
- 10.5 Symmetry in Molecular Spectroscopy
- 10.6 Statistical Weight
- 10.7 Selection Rules
- 10.8 Rabi Frequency
- 10.9 Linear and Nonlinear Spectroscopies
- 10.10 One- and Multi-Photon Transitions

二. 教科書: “Quantum Chemistry” (5th edition/2000)
by I. N. Levine (Prentice Hall)

三. 成績評量: 期中考, 期末考, 及平常作業。

四. 化圖指定參考書 (reserved books)

1. 書名: Quantum Chemistry
作者: I. N. Levin
出版者: Prentice Hall
版次/出版年: 5th Edition / 2000
2. 書名: Quantum Mechanics, Volume I & II
作者: C. Cohen-Tannoudji
出版者: John Wiley & Sons
版次/出版年: 1977
3. 書名: Quantum Mechanics (Nonrelativistic Theory)
作者: L. D. Landau and E. M. Lifshitz
出版者: Pergamon Press
版次/出版年: 1977
4. 書名: Physical Chemistry: A Molecular Approach
作者: Donald A. McQuarrie / John D. Simon
出版者: University Science Books
版次/出版年: 1997