This is a text dealing with the basics of quantum mechanics and electronic structure theory. It provides an introduction to molecular spectroscopy and to the subject of molecular dynamics.

1: The Basic Tools of Quantum Mechanics

\[ E_n^{(1)} = \langle \phi_n | H_1 | \phi_n \rangle \]

\[ c_{nk}^{(1)} = \frac{\langle \phi_k | H_1 | \phi_n \rangle}{E_n^{(0)} - E_k^{(0)}} \]

\[ E_n^{(2)} = \sum_{k \neq n} \frac{|\langle \phi_k | H_1 | \phi_n \rangle|^2}{E_n^{(0)} - E_k^{(0)}} \]

2: Approximation Methods

3: Nuclear Motion

4: Atomic Orbitals
constructive orbital overlap

- 6: Quantum Mechanics in Reactions

- 7: Further Characterization of Molecular Orbitals

\[
\begin{pmatrix}
B_{1,1} & B_{1,2} & \cdots & B_{1,N} \\
B_{2,1} & B_{2,2} & \cdots & B_{2,N} \\
\vdots & \vdots & \ddots & \vdots \\
B_{N,1} & B_{N,2} & \cdots & B_{N,N}
\end{pmatrix}
\]
9: Symmetry of Electronic Wavefunctions

10: Angular Momentum and Group Symmetries of Electronic Wavefunctions

\[ \langle \Psi | \hat{F} | \Psi \rangle = \sum_{i=1}^{N} \langle \phi_i | \hat{f} | \phi_i \rangle, \]
\[ \langle \Psi | \hat{F} | \Psi^p_m \rangle = \langle \phi_m | \hat{f} | \phi_p \rangle, \]
\[ \langle \Psi | \hat{F} | \Psi_{ran} \rangle = 0. \]

11: Evaluating the Matrix Elements of N-electron Wavefunctions

12: Quantum Mechanical Picture of Bond Making and Breaking Reactions

13: Molecular Rotation and Vibration
14: Time-dependent Quantum Dynamics

15: Spectroscopy

16: Collisions and Scattering

17: Higher Order Corrections to Electronic Structure
18: Multiconfiguration Wavefunctions

19: Multi-Determinant Wavefunctions

20: Response Theory

No image available

21: Problem Sets

22: Problems
Contributors

- [Jack Simons](#) (Henry Eyring Scientist and Professor of Chemistry, U. Utah) [Telluride Schools on Theoretical Chemistry](#) and [Jeff A. Nichols](#) (Oak Ridge National Laboratory)