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.

• Front Matter

• 1: The Basic Tools of Quantum Mechanics

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

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

• 2: Approximation Methods

• 3: Nuclear Motion
4: Atomic Orbitals

5: Molecular Orbitals

6: Quantum Mechanics in Reactions

7: Further Characterization of Molecular Orbitals
8: Electronic Configurations

\[ \mathbf{B} = \begin{pmatrix} B_{1,1} & B_{1,2} & \cdots & B_{1,N} \\ B_{2,1} & B_{2,2} & \cdots & B_{2,N} \\ \vdots & \vdots & \ddots & \vdots \\ B_{N,1} & B_{N,2} & \cdots & B_{N,N} \end{pmatrix} \]

9: Symmetry of Electronic Wavefunctions

10: Angular Momentum and Group Symmetries of Electronic Wavefunctions

\[ \langle \Psi | \hat{F} | \Psi \rangle = \sum_{i=1}^{N} \langle \phi_i | \hat{f} | \phi_i \rangle, \]

\[ \langle \Psi | \hat{F} | \Psi_{m}^{\parallel} \rangle = \langle \phi_m | \hat{f} | \phi_p \rangle, \]

\[ \langle \Psi | \hat{F} | \Psi_{\text{ran}}^{\parallel} \rangle = 0. \]

11: Evaluating the Matrix Elements of N-electron Wavefunctions

\[ \begin{array}{c}
\begin{array}{c}
A \rightarrow B \\
A \leftrightarrow B
\end{array}
\end{array} \rightarrow \begin{array}{c}
\begin{array}{c}
A^+ + B^- \\
A^- + B^+
\end{array}
\end{array} \]
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
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