CHAPTER OVERVIEW

1: The Basics of Quantum Mechanics

Learning Objectives

In this Chapter, you should have learned about the following things:

- Why quantum mechanics is needed; that is, what things classical mechanics does not describe correctly. How quantum and classical descriptions can sometimes agree and when they will not. How certain questions can only be asked when classical mechanics applies, not when quantum mechanics is needed.
- The Schrödinger equation, operators, wave functions, eigenvalues and eigenfunctions and their relations to experimental observations.
- Time propagation of wave functions.
- Free particle motion and corresponding eigenfunctions in one, two, and three dimensions and the associated energy levels, and the relevance of these models to various chemistry issues.
- Action quantization and the resulting semi-classical wave functions and how this point of view offers connections between classical and quantum perspectives.

In this portion of the text, most of the topics that are appropriate to an undergraduate reader are covered. Many of these subjects are subsequently discussed again in Chapter 5, where a broad perspective of what theoretical chemistry is about is offered. They are treated again in greater detail in Chapters 6-8 where the three main disciplines of theory, electronic structure, chemical dynamics, and statistical mechanics, are covered in depth appropriate to a graduate-student reader.

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