

CHAPTER OVERVIEW

2: Particle in a Box

In this chapter, we will develop the theoretical problem of a particle in a box. The purpose here is to explore the capabilities of quantum mechanics and see how some of the mathematical machinery works. The reason for "kicking the tires" of quantum theory with this particular problem is that the math is fairly simple (at least by comparison!) and the results are relatively easy to interpret. After developing a toolbox of methods in this chapter, we can focus more on the results as applied to more complex problems of greater chemical importance.

- [2.1: Background](#)
- [2.2: The Postulates of Quantum Mechanics](#)
- [2.3: The One-Dimensional Particle in a Box](#)
- [2.4: The Tools of Quantum Mechanics](#)
- [2.5: Superposition and Completeness](#)
- [2.6: Problems in Multiple Dimensions](#)
- [2.7: The Free Electron Model](#)
- [2.8: Entanglement and Schrödinger's Cat](#)
- [2.9: References](#)
- [2.10: Vocabulary and Concepts](#)
- [2.11: Problems](#)

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