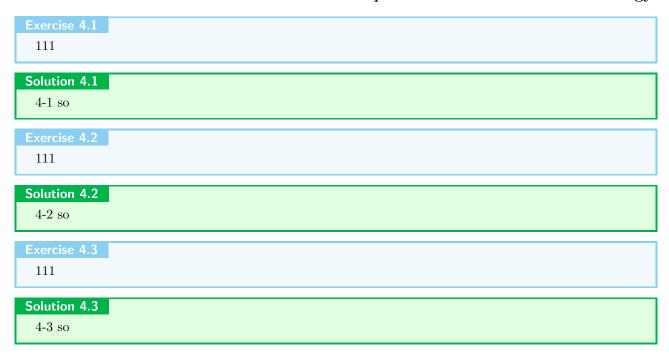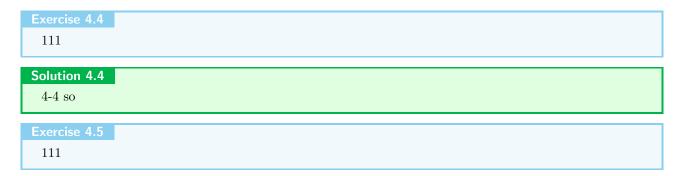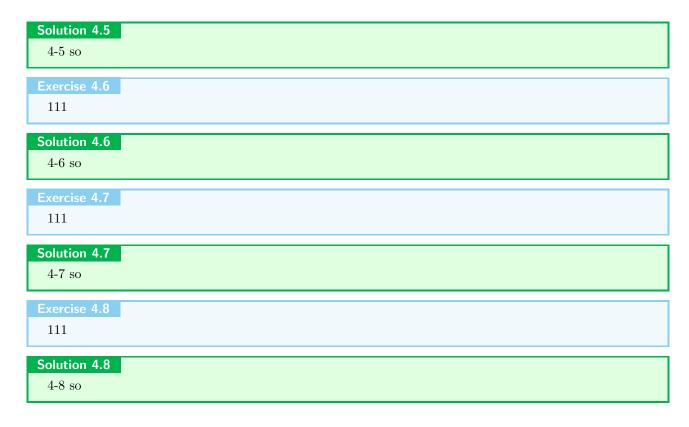# CHAPTER 4

Configuration Interaction

4.1 Multiconfigurational Wave Functions and the Structure of the Full CI Matrix

4.1.1 Intermediate Normalization and an Expression for the Correlation Energy

> **Exercise 4.1**
> 111

> **Solution 4.1**
> 4-1 so

> **Exercise 4.2**
> 111

> **Solution 4.2**
> 4-2 so

> **Exercise 4.3**
> 111

> **Solution 4.3**
> 4-3 so

4.2 Doubly Excited CI

4.3 Some Illustrative Calculations

4.4 Natural Orbitals and the One-Particle Reduced Density Matrix

> **Exercise 4.4**
> 111

> **Solution 4.4**
> 4-4 so

> **Exercise 4.5**
> 111

Solution 4.5

4-5 so

Exercise 4.6

111

Solution 4.6

4-6 so

Exercise 4.7

111

Solution 4.7

4-7 so

Exercise 4.8
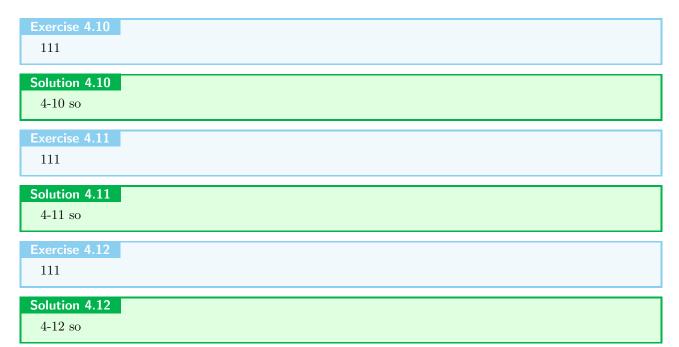
111

Solution 4.8

4-8 so

4.5   The Multiconfiguration Self-Consistent Field (MCSCF) and Generalized Valence Bond (GVB) Methods

Exercise 4.9

111

Solution 4.9

4-9 so

4.6   Truncated CI and the Size-Consistency Problem

Exercise 4.10

111

Solution 4.10

4-10 so

Exercise 4.11

111

Solution 4.11

4-11 so

Exercise 4.12

111

Solution 4.12

4-12 so

Exercise 4.13

111

Solution 4.13

4-13 so

Exercise 4.14

111

Solution 4.14

4-14 so

Exercise 4.15

111

Solution 4.15

4-15 so