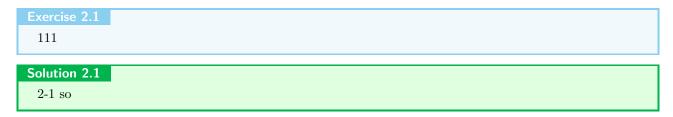
CHAPTER 2

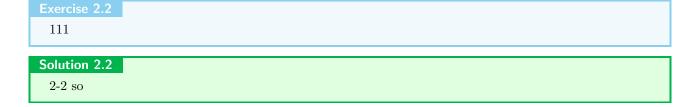
Many Electron Wave Functions and Operators

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2.1	The	Electron	1 Prob	IAM
4. L	T 11C		1 1 100	\mathbf{L}

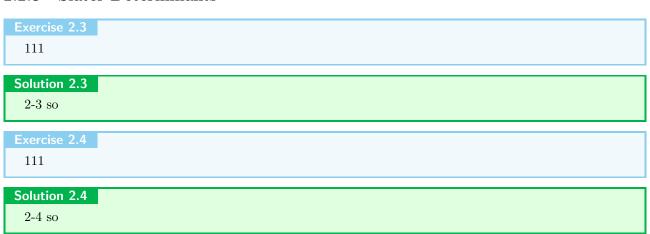
- 2.1.1 Atomic Units
- 2.1.2 The Born-Oppenheimer Approximation
- 2.1.3 The Antisymmetry or Pauli Exclusion Principle
- 2.2 Orbitals, Slater Determinants, and Basis Functions
- 2.2.1 Spin Orbitals and Spatial Orbitals



2.2.2 Hartree Products



2.2.3 Slater Determinants



Exercise 2.5	
111	
Solution 2.5	
2-5 so	

- 2.2.4 The Hartree-Fock Approximation
- 2.2.5 The Minimal Basis H₂ Model

```
Exercise 2.6 Show that \psi_1 and \psi_2 form an orthonormal set.

Solution 2.6 2-6 so
```

- 2.2.6 Excited Determinants
- 2.2.7 Form of the Exact Wave Function and Configuration Interaction

```
Exercise 2.7
111

Solution 2.7
2-7 so
```

- 2.3 Operators and Matrix Elements
- 2.3.1 Minimal Basis H₂ Matrix Elements

```
Exercise 2.8
111

Solution 2.8
2-8 so

Exercise 2.9
111

Solution 2.9
2-9 so
```

- 2.3.2 Notations for One- and Two-Electron Integrals
- 2.3.3 General Rules for Matrix Elements

```
Exercise 2.10
111

Solution 2.10
2-10 so
```

Exercise 2.11 111	
Solution 2.11 2-11 so	
Exercise 2.12 111	
Solution 2.12 2-12 so	
Exercise 2.13 111	
Solution 2.13 2-13 so	
Exercise 2.14 111	
2-14 so	

2.3.4 Derivation of the Rules for Matrix Elements

```
Exercise 2.15
111

Solution 2.15
2-15 so

Exercise 2.16
111

Solution 2.16
2-16 so
```

2.3.5 Transition from Spin Orbitals to Spatial Orbitals

```
Exercise 2.17
111

Solution 2.17
2-17 so

Exercise 2.18
111

Solution 2.18
2-18 so
```

2.3.6 Coulomb and Exchange Integrals

Exercise 2.19

111

Solution 2.19

2-19 so

Exercise 2.20

Show that for *real* spatial orbitals

$$K_{ij} = (ij|ij) = (ji|ji) = \langle ii|jj\rangle = \langle jj|ii\rangle.$$

Solution 2.20

2-20 so

Exercise 2.21

111

Solution 2.21

2-21 so

Exercise 2.22

111

Solution 2.22

2-22 so

2.3.7 Pseudo-Classical Interpretation of Determinantal Energies

Exercise 2.23

111

Solution 2.23

2-23 so

2.4 Second Quantization

2.4.1 Creation and Annihilation Operators and Their Anticommutation Relations

Exercise 2.24

111

Solution 2.24

2-24 so

Exercise 2.25

111

Solution 2.25

2-25 so

Exercise 2.26			
Solution 2.26 2-26 so			
Exercise 2.27			
Solution 2.27 2-27 so			
Exercise 2.28			
Solution 2.28 2-28 so			

2.4.2 Second-Quantized Operators and Their Matrix Elements

```
Exercise 2.29
111

Solution 2.29
2-29 so

Exercise 2.30
111

Solution 2.30
2-30 so

Exercise 2.31
111

Solution 2.31
2-31 so
```

2.5 Spin-Adapted Configurations

2.5.1 Spin Operators

```
Exercise 2.32
111

Solution 2.32
2-32 so

Exercise 2.33
111
```

Solution 2.33 2-33 so	
Exercise 2.34	
Solution 2.34 2-34 so	
Exercise 2.35	
Solution 2.35 2-35 so	
Exercise 2.36	
Solution 2.36 2-36 so	
Exercise 2.37	
Solution 2.37 2-37 so	
2.5.2 Restric	cted Determinants and Spin-Adapted Configurations

2.5.2 Restricted Determinants and Spin-Adapted Configurations

```
Solution 2.38
2-38 so

Exercise 2.38
111

Solution 2.39
2-39 so

Exercise 2.39
111

Solution 2.40
2-40 so
```

2.5.3 Unrestricted Determinants

```
Exercise 2.40
111

Solution 2.41
2-41 so
```