CHAPTER 5

Pair and Coupled-Pair Theories

5.1 The Independent Electron Pair Approximation (IEPA)

Exercise 5.1

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Solution 5.1

5-1 so

Exercise 5.2

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Solution 5.2

5-2 so

Exercise 5.3

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Solution 5.3

5-3 so

5.1.1 Invariance under Unitary Transformations: An Example

Exercise 5.4

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Solution 5.4

5-4 so

Exercise 5.5

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Solution 5.5

5-5 so

Exercise 5.6

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Solution 5.6

5-6 so

Exercise 5.7

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Solution 5.7

5-7 so

Exercise 5.8

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Solution 5.8

5-8 so

Exercise 5.9

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Solution 5.9

5-9 so

Exercise 5.10

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Solution 5.10

5-10 so

5.1.2 Some Illustrative Calculations

5.2 Coupled-Pair Theories

5.2.1 The Coupled Cluster Approximation (CCA)

5.2.2 The Cluster Expansion of the Wave Function

Exercise 5.11

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Solution 5.11

5-11 so

5.2.3 Linear CCA and the Coupled Electron Pair Approximation (CEPA)

Exercise 5.12

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Solution 5.12

5-12 so

5.2.4 Some Illustrative Calculations

5.3 Many-Electron Theories with Single Particle Hamiltonians

Exercise 5.13

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Solution 5.13

5-13 so

5.3.1 The Relaxation Energy via CI, IEPA, CEPA, and CCA

Exercise 5.14

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Solution 5.14

5-14 so

Exercise 5.15

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Solution 5.15

5-15 so

5.3.2 The Resonance Energy of Polyenes in Hückel Theory

Exercise 5.16

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Solution 5.16

5-16 so

Exercise 5.17

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Solution 5.17

5-17 so

Exercise 5.18

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Solution 5.18

5-18 so

Exercise 5.19

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Solution 5.19

5-19 so

Exercise 5.20

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Solution 5.20

5-20 so

Exercise 5.21

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Solution 5.21

5-21 so