the Manual Solution of Modern Quantum Chemistry(Szabo,1982)

supplyed by 霜城雪 and 超锂化雪

2021.11.10-

目录

Chapter 1 Mathematical Review

exercise 1.1

Chapter 2 Many Electron Wave Functions and Operators

exercise 2.1

$$\langle \chi_{2i-1}|\chi_{2j-1}\rangle = \langle \psi_i^{\alpha}|\psi_j^{\beta}\rangle = \delta_{ij}\cdot 1 = \delta_{ij}\ ;\ \langle \chi_{2i}|\chi_{2j}\rangle = \langle \psi_i^{\beta}|\psi_j^{\beta}\rangle = \delta_{ij}\cdot 1 = \delta_{ij}.$$

$$\langle \chi_{2i-1}|\chi_{2j}\rangle = \langle \psi_i^{\alpha}|\psi_j^{\beta}\rangle = \delta_{ij}\cdot 0 = 0\ ;\ \langle \chi_{2i}|\chi_{2j-1}\rangle = \langle \psi_i^{\beta}|\psi_j^{\alpha}\rangle = \delta_{ij}\cdot 0 = 0.$$

exercise 2.2

$$\mathscr{H}\psi^{HP} = \sum_{i=1}^{N} h(i)\psi^{HP} = \sum_{i=1}^{N}\varepsilon_i\psi^{HP} = \Big(\sum_{i=1}^{N}\varepsilon_i\Big)\psi^{HP}$$

$$\therefore E = \sum_{i=1}^{N}\varepsilon_i.$$

exercise 2.3

$$\begin{aligned}\langle\Psi|\Psi\rangle = &\int_{\Omega_1}\mathrm{d}x_1\int_{\Omega_2}\mathrm{d}x_2\frac{1}{\sqrt{2}}[\chi_i(1)\chi_j(2)-\chi_j(1)\chi_i(2)]^*\frac{1}{\sqrt{2}}[\chi_i(1)\chi_j(2)-\chi_j(1)\chi_i(2)]\\ =&\frac{1}{2}(1+0+0+1) = 1.\end{aligned}$$

exercise 2.4

$$
\begin{aligned}
&\mathscr{H}\frac{1}{\sqrt{2}}(\chi_i(1)\chi_j(2)-\chi_j(1)\chi_i(2))\\
=&h(1)\frac{1}{\sqrt{2}}(\chi_i(1)\chi_j(2)-\chi_j(1)\chi_i(2))+h(2)\frac{1}{\sqrt{2}}(\chi_i(1)\chi_j(2)-\chi_j(1)\chi_i(2))\\
=&\varepsilon_i\frac{1}{\sqrt{2}}\chi_i(1)\chi_j(2)-\varepsilon_j\frac{1}{\sqrt{2}}\chi_j(1)\chi_i(2)+\frac{1}{\sqrt{2}}\varepsilon_j\chi_i(1)\chi_j(2)-\frac{1}{\sqrt{2}}\varepsilon_i\chi_j(1)\chi_i(2)\\
=&(\varepsilon_i+\varepsilon_j)\frac{1}{\sqrt{2}}(\chi_i(1)\chi_j(2)-\chi_j(1)\chi_i(2)).
\end{aligned}
$$

从而$|\Psi^{HP}\rangle$能量为$\varepsilon_i+\varepsilon_j$.

exercise 2.5

$$
\begin{aligned}
&\langle K|L\rangle=\langle ij|kl\rangle\\
=&\frac{1}{2}\int_{\Omega_1}\mathrm{d}x_1\int_{\Omega_2}\mathrm{d}x_2[\chi_i(1)\chi_j(2)-\chi_j(1)\chi_i(2)]^*[\chi_k(1)\chi_l(2)-\chi_l(1)\chi_k(2)]\\
=&\frac{1}{2}[\langle ij|kl\rangle-\langle ij|lk\rangle-\langle ji|kl\rangle+\langle ji|lk\rangle]\\
=&\frac{1}{2}[\delta_{ik}\delta_{jl}-\delta_{il}\delta_{jk}-\delta_{jk}\delta_{il}+\delta_{jl}\delta_{ik}]\\
=&\delta_{ik}\delta_{jl}-\delta_{jk}\delta_{il}\equiv\delta_{ij}^{kl}.
\end{aligned}
$$

推广：我们知道，在平直空间张量分析中，$\delta_{ij}^{kl}\equiv\delta_{ik}\delta_{jl}-\delta_{jk}\delta_{il}$。故而大胆猜测有

$$\langle\chi_{i_1}\chi_{i_2}\cdots\chi_{i_N}|\chi_{j_1}\chi_{j_2}\cdots\chi_{j_N}\rangle=\delta_{i_1i_2\cdots i_N}^{j_1j_2\cdots j_N}.$$

证明：

$$
\begin{aligned}
&\langle i_1 i_2 \cdots i_N | j_1 j_2 \cdots j_N \rangle \\
=&\frac{1}{N!}\sum_{i_1 i_2 \cdots i_N}\sum_{j_1 j_2 \cdots j_N}(-1)^{\tau(i_1 i_2 \cdots i_N)}(-1)^{\tau(j_1 j_2 \cdots j_N)}\delta_{i_1 i_2 \cdots i_N}^{j_1 j_2 \cdots j_N} \\
=&\sum_{i_1 i_2 \cdots i_N}(-1)^{\tau(i_1 i_2 \cdots i_N)+\tau(j_1 j_2 \cdots j_N)}\delta_{i_1}^{j_1}\delta_{i_2}^{j_2}\cdots\delta_{i_N}^{j_N} \\
=&\delta_{i_1 i_2 \cdots i_N}^{j_1 j_2 \cdots j_N}.
\end{aligned}
$$

exercise 2.6

$$
\begin{aligned}
&\langle \psi_1 | \psi_1 \rangle \\
&\quad=\frac{1}{2(1+S_{12})}\int_{\Omega_{r_1}}\mathrm{d}r_1\int_{\Omega_{r_2}}\mathrm{d}r_2(\phi_1+\phi_2)^*(\phi_1+\phi_2) \\
&\quad=\frac{1}{2(1+S_{12})}(1+S_{12}+S_{12}+1)=1.
\end{aligned}
$$

同理

$$\langle \psi_2 | \psi_2 \rangle = 1.$$

$$
\begin{aligned}
&\langle \psi_1 | \psi_2 \rangle \\
&\quad=\frac{1}{2\sqrt{1-S_{12}^2}}\int_{\Omega_{r_1}}\mathrm{d}r_1\int_{\Omega_{r_2}}\mathrm{d}r_2(\phi_1+\phi_2)^*(\phi_1-\phi_2) \\
&\quad=\frac{1}{2\sqrt{1-S_{12}^2}}(1-S_{12}+S_{12}-1)=0.
\end{aligned}
$$

故ψ_1与ψ_2形成一个标准正交基.

exercise 2.7

苯分子有42个电子(1个碳原子提供6个，1个氢原子提供1个)，却有36个原子轨道(1个碳原子提供1s, 2s及2p三种五个轨道从，1个氢原子提供1s一种一个轨道)，考虑到一个原子轨道可容纳一对(自旋相反的)电子，由电子的不可分辨性，有$C_{72}^{42}=1.64\times10^{20}$种方法，此即Full CI中行列式总数.

单激发态需选1个电子填充另一组空轨道，从而有$C_{42}^{1}C_{30}^{1}\doteq 1260$种.

类似地，双激发态有$C_{32}^{2}C_{40}^{2}\doteq 3.74\times10^{5}$种.

exercise 2.8

$$\langle\psi_{12}^{34}|\vartheta_1|\psi_{12}^{34}\rangle = \langle\psi_{12}^{34}|h(1)|\psi_{12}^{34}\rangle + \langle\psi_{12}^{34}|h(2)|\psi_{12}^{34}\rangle.$$

$$\begin{aligned}
&\langle 2\bar{2}|h(1)|2\bar{2}\rangle \\
=&\frac{1}{2}\int_{\Omega_1}\mathrm{d}x_1\int_{\Omega_2}\mathrm{d}x_2[\chi_3(1)\chi_4(2)-\chi_4(1)\chi_3(2)]^*h(1)[\chi_3(1)\chi_4(2)-\chi_4(1)\chi_3(2)] \\
=&\frac{1}{2}\int_{\Omega_1}\mathrm{d}x_1[\chi_3^*(1)h(1)\chi_3(1)+\chi_4^*(1)h(1)\chi_4(1)] \\
=&\frac{1}{2}[\langle 3|h|3\rangle+\langle 4|h|4\rangle],
\end{aligned}$$

同理,

$$\langle 2\bar{2}|h(2)|2\bar{2}\rangle = \frac{1}{2}[\langle 3|h|3\rangle+\langle 4|h|4\rangle].$$

$$\therefore \langle 2\bar{2}|\vartheta_1|2\bar{2}\rangle = \langle 2\bar{2}|h(1)|2\bar{2}\rangle + \langle 2\bar{2}|h(2)|2\bar{2}\rangle = \langle 3|h|3\rangle+\langle 4|h|4\rangle.$$

而

$$\langle 2\bar{2}|h(1)|\psi_0\rangle = \frac{1}{2}\int_{\Omega_1}\mathrm{d}x_1\int_{\Omega_2}\mathrm{d}x_2[\chi_3(1)\chi_4(2)-\chi_3(2)\chi_4(1)]^*h(1)[\chi_1(1)\chi_2(2)-\chi_2(1)\chi_1(1)] = 0.$$

同理

$$\langle\psi_{12}^{34}|h(2)|\psi_0\rangle = 0.$$

从而

$$\langle\psi_{12}^{34}|\vartheta_1|\psi_0\rangle = 0.$$

同理

$$\langle\psi_0|\vartheta_1|\psi_{12}^{34}\rangle = 0.$$

exercise 2.9

同教材方法推导即可. 注意重积分的值和积分变量无关，允许交换积分

傀标.

$$
\begin{aligned}
&\langle\psi_0|\vartheta_2|\psi_{12}^{34}\rangle\\
=&\frac{1}{2}\int_{\Omega_1}\mathrm{d}x_1\int_{\Omega_2}\mathrm{d}x_2[\chi_1(1)\chi_2(2)-\chi_2(1)\chi_1(2)]^*r_{12}^{-1}[\chi_3(1)\chi_4(2)-\chi_4(1)\chi_3(2)]\\
=&\frac{1}{2}\int_{\Omega_1}\mathrm{d}x_1\int_{\Omega_2}\mathrm{d}x_2[\chi_1^*(1)\chi_2^*(2)r_{12}^{-1}\chi_3(1)\chi_4(2)-\chi_1^*(1)\chi_2^*(2)r_{12}^{-1}\chi_3(2)\chi_4(1)-\chi_2^*(1)\chi_1^*(2)r_{12}^{-1}\chi_3(1)\chi_4(2)-\\
=&\frac{1}{2}[\langle 12|34\rangle+\langle 21|43\rangle-\langle 12|43\rangle-\langle 21|34\rangle]\\
=&\frac{1}{2}[\langle 12|34\rangle+\langle 12|34\rangle-\langle 12|43\rangle-\langle 12|43\rangle]\\
=&\langle 12|34\rangle-\langle 12|43\rangle.
\end{aligned}
$$

$$\therefore\langle\psi_0|\mathscr{H}|\psi_{12}^{34}\rangle=\langle\psi_0|\vartheta_1|\psi_{12}^{34}\rangle+\langle\psi_0|\vartheta_2|\psi_{12}^{34}\rangle.$$

由练习2.8得

$$\langle\psi_0|\vartheta_1|\psi_{12}^{34}\rangle=0,\ \therefore\langle\psi_0|\mathscr{H}|\psi_{12}^{34}\rangle=\langle 12|34\rangle-\langle 12|43\rangle.$$

同理

$$\langle\psi_{12}^{34}|\mathscr{H}|\psi_0\rangle=\langle 34|12\rangle-\langle 34|21\rangle.$$

由教材知

$$\langle\psi_0|\mathscr{H}|\psi_0\rangle=\langle 1|h|1\rangle+\langle 2|h|2\rangle+\langle 12|12\rangle-\langle 12|21\rangle.$$

同理

$$\langle\psi_{12}^{34}|\mathscr{H}|\psi_0\rangle=\langle\psi_{12}^{34}|\vartheta_1|\psi_{12}^{34}\rangle+\langle\psi_{12}^{34}|\vartheta_2|\psi_{12}^{34}\rangle=\langle 3|h|3\rangle+\langle 4|h|4\rangle+\langle 34|34\rangle-\langle 34|43\rangle.$$

exercise 2.10

先推导式(2.109a)与式(2.109.b), 再以之推导他式.

$$\langle mm||mm\rangle=\langle mm|mm\rangle-\langle mm|mm|rangle=0.$$

同理, $\langle nn||nn\rangle=0$. 式(2.109a)得证.

$$\langle mn||mn\rangle=\langle mn|mn\rangle-\langle mn|nm\rangle=\langle nm|nm\rangle-\langle nm|mn\rangle=\langle nm||nm\rangle.$$

式(2.109b)得证. 从式(2.107)推导式(2.110)如下

$$\begin{aligned}
&\langle K|\mathscr{H}|K\rangle \\
&=\sum_{m}^{N}\langle m|h|m\rangle+\frac{1}{2}\sum_{m}^{N}\sum_{n}^{N}\langle mn||mn\rangle \\
&=\sum_{m}^{N}\langle m|h|m\rangle+\sum_{n>m}^{N}\sum_{m}^{N}\langle mn||mn\rangle \\
&=\sum_{m}^{N}\langle m|h|m\rangle+\sum_{n>m}^{N}\sum_{m}^{N}[\langle mn|mn\rangle-\langle mn|nm\rangle] \\
&=\sum_{m}^{N}\langle m|h|m\rangle+\sum_{n>m}^{N}\sum_{m}^{N}([mm|nn]-[mn|nm]).
\end{aligned}$$

exercise 2.11

利用练习2.10结论立得

$$\langle K|\mathscr{H}|K\rangle=\langle 1|h|1\rangle+\langle 2|h|2\rangle+\langle 3|h|3\rangle+\langle 12||12\rangle+\langle 13||13\rangle+\langle 23||23\rangle.$$

exercise 2.12

利用矩阵元计算的一般规则计算即可. 教材式(2.111)-(2.114)已解释H_2最小基中$\langle\psi_0|\mathscr{H}|\psi_0\rangle$由来. 而

$$\langle\psi_0|\vartheta_1|\psi_{12}^{34}\rangle=0,\ \langle\psi_0|\vartheta_2|\psi_{12}^{34}\rangle=\langle 12||34\rangle,$$

$$\therefore\langle\psi_0|\mathscr{H}|\psi_{12}^{34}\rangle=\langle\psi_0|\vartheta_1|\psi_{12}^{34}\rangle+\langle\psi_0|\vartheta_2|\psi_{12}^{34}\rangle=\langle 12||34\rangle.$$

同理, $\langle\psi_{12}^{34}|\mathscr{H}|\psi_0\rangle=\langle 34||12\rangle$, 而$\langle\psi_{12}^{34}|\vartheta_1|\psi_{12}^{34}\rangle=\langle 3|h\,3\rangle+\langle 4|h\,4\rangle$, $\langle\psi_{12}^{34}|\vartheta_2|\psi_{12}^{34}\rangle=\langle 34||34\rangle$,

$$\therefore\langle\psi_{12}^{34}|\mathscr{H}|\psi_{12}^{34}\rangle=\langle\psi_{12}^{34}|\vartheta_1|\psi_{12}^{34}\rangle+\langle\psi_{12}^{34}|\vartheta_2|\psi_{12}^{34}\rangle=\langle 3|h|3\rangle+\langle 4|h|4\rangle+\langle 34||34\rangle.$$

exercise 2.13

利用规则计算即可. 只是题目叙述不严谨, ab及rs应是紧邻的两轨道, 否则不能应用表2.3.

当$a \neq b, r \neq s$时, $\langle \psi_a^r | \vartheta_1 | \psi_b^s \rangle$中有两电子不同, 从而$\langle \psi_a^r | \vartheta_1 | \psi_b^s \rangle = 0$;

当$a = b, r \neq s$时, $\langle \psi_a^r | \vartheta_1 | \psi_b^s \rangle = \langle \psi_a^r | \vartheta_1 | \psi_a^s \rangle$中有一电子不同, 从而$\langle \psi_a^r | \vartheta_1 | \psi_a^s \rangle = \langle r | h | s \rangle$;

当$a \neq b, r = s$时, $\langle \psi_a^r | \vartheta_1 | \psi_b^s \rangle = \langle \psi_a^r | \vartheta_1 | \psi_b^r \rangle = \langle \cdots \chi_r \cdots \chi_b \cdots | \vartheta_1 | \cdots \chi_a \cdots \chi_r \cdots = -\langle \cdots \chi_b \cdots \chi_r \cdots | \vartheta_1 | \cdots \chi_a \cdots \chi_r \cdots$, 从而$\langle \psi_a^r | \vartheta_1 | \psi_b^s \rangle = -\langle b | h | a \rangle$;

当$a = b, r = s$时, $\langle \psi_a^r | \vartheta_1 | \psi_b^s \rangle = \langle \psi_a^r | \vartheta_1 | \psi_a^r \rangle = \sum_c^N \langle c | h | c \rangle - \langle a | h | a \rangle + \langle r | h | r \rangle$.

综上, 知原命题成立.

exercise 2.14

用定义验证即可, 带撇号的求和对除去a以外的所有项求和, 否则是对所有项求和.

$$
{}^N E_0 -^{N-1} E_0 = \Big[\sum_b^N \langle b | h | b \rangle + \frac{1}{2} \sum_c^N \sum_d^N \langle cd || cd \rangle \Big] - \Big[\sum_b^N{}' \langle b | h | b \rangle + \frac{1}{2} \sum_c^N{}' \sum_d^N{}' \langle cd || cd \rangle \Big]
$$

$$
= \langle a | h | a \rangle + \frac{1}{2} \sum_c^N{}' \langle ca \| ca \rangle + \frac{1}{2} \sum_d^N{}' \langle ad \| ad \rangle + \langle aa \| aa \rangle = \langle a | h | a \rangle + \sum_b^N \langle ab \| ab \rangle.
$$

exercise 2.15

$$
\begin{aligned}
&\mathscr{H}|\chi_i\chi_j\cdots\chi_k\rangle\\
=&\mathscr{H}\frac{1}{\sqrt{N!}}\sum_{i_1i_2\cdots i_N}(-1)^{\tau(i_1i_2\cdots i_N)}\chi_{i_1}(1)\chi_{i_2}(2)\cdots\chi_{i_N}(N)\\
=&\sum_{i=1}^{N}h(i)\frac{1}{\sqrt{N!}}\sum_{i_1i_2\cdots i_N}(-1)^{\tau(i_1i_2\cdots i_N)}\chi_{i_1}(1)\chi_{i_2}(2)\cdots\chi_{i_N}(N)\\
=&\sum_{i=1}^{N}\frac{1}{\sqrt{N!}}\sum_{i_1i_2\cdots i_N}(-1)^{\tau(i_1i_2\cdots i_N)}h(i)\chi_{i_1}(1)\chi_{i_2}(2)\cdots\chi_{i_N}(N)\\
=&\frac{1}{\sqrt{N!}}\sum_{i=1}^{N}\sum_{i_1i_2\cdots i_N}(-1)^{\tau(i_1i_2\cdots i_N)}\varepsilon(i)\chi_{i_1}(1)\chi_{i_2}(2)\cdots\chi_{i_N}(N)\\
=&\sum_{i=1}^{N}\varepsilon_i\frac{1}{\sqrt{N!}}\sum_{i_1i_2\cdots i_N}(-1)^{\tau(i_1i_2\cdots i_N)}\chi_{i_1}(1)\chi_{i_2}(2)\cdots\chi_{i_N}(N)\\
=&\Big(\sum_{i=1}^{N}\varepsilon_i\Big)|\chi_i\chi_j\cdots\chi_k\rangle.
\end{aligned}
$$

exercise 2.16

由练习2.15. $\mathscr{H}|\chi_i\chi_j\cdots\chi_k\rangle=\Big(\sum_{i=1}^{N}\varepsilon_i\Big)|\chi_i\chi_j\cdots\chi_k\rangle$,
由练习2.2. $\mathscr{H}|K^{HP}\rangle=\Big(\sum_{i=1}^{N}\varepsilon_i\Big)|K^{HP}\rangle$.

$$
\begin{aligned}
\therefore \langle K|\mathscr{H}|L\rangle=&\sum_{i=1}^{N}\varepsilon_i\langle K|L\rangle\\
=&\sum_{i=1}^{N}\varepsilon_i\frac{1}{\sqrt{N!}}\sum_{i_1i_2\cdots i_N}(-1)^{\tau(i_1i_2\cdots i_N)}\langle i_1i_2\cdots i_N|L\rangle\\
=&\sum_{i=1}^{N}\varepsilon_i\frac{1}{\sqrt{N!}}\sum_{i_1i_2\cdots i_N}(-1)^{\tau(i_1i_2\cdots i_N)}\delta^{L}_{i_1i_2\cdots i_N}.
\end{aligned}
$$

若$|K^{HP}\rangle$与$|L\rangle$不相同, 即$\langle K^{HP}|L\rangle=0$. 则由相同种类轨道构成的$|K\rangle$必然有$\langle K|L\rangle=0$; 反之, 若$\langle K^{HP}|L\rangle=1$或$\langle K^{HP}|L\rangle=-1$, 则$\sum_{i_1i_2\cdots i_N}(-1)^{\tau(i_1i_2\cdots i_N)}\delta^{L}_{i_1i_2\cdots i_N}$中

有且仅有一项为1, 其余为0，从而

$$\langle K|\mathscr{H}|L\rangle = \frac{1}{\sqrt{N!}}\sum_{i=1}^{N}\varepsilon_i\langle K_i^{HP}|L\rangle = \frac{1}{\sqrt{N!}}\langle K^{HP}|L\rangle.$$

证明单电子积分的运算规则的可参考个人读后感2.3.4节，有详细同思路证明。

exercise 2.17

依次化简练习2.9中的矩阵元，结果为

$$\begin{aligned}
&H(1,1) = \langle 1|h|1\rangle + \langle 2|h|2\rangle + \langle 12|12\rangle + \langle 12|21\rangle \\
&= [1|h|1] + [\bar{1}|h|\bar{1}] + [11|\bar{1}\bar{1}] + [1\bar{1}|\bar{1}1] \\
&= (1|h|1) + (1|h|1) + (11|11) = 2(1|h|1) + (11|11).
\end{aligned}$$

$$H(1,2) = \langle 12|34\rangle - \langle 12|43\rangle = [12|\bar{1}\bar{2}] - [1\bar{2}|\bar{1}2] = (12|12).$$

$$H(2,1) = \langle 34|12\rangle - \langle 34|21\rangle = [21|\bar{2}\bar{1}] - [2\bar{1}|\bar{2}1] = (21|21).$$

$$\begin{aligned}
&H(2,2) = \langle 3|h|3\rangle + \langle 4|h|4\rangle + \langle 34|34\rangle - \langle 34|43\rangle \\
&= [2|h|2] + [\bar{2}|h|\bar{2}] + [22|\bar{2}\bar{2}] - [2\bar{2}|\bar{2}2] \\
&= (2|h|2) + (2|h|2) + (22|22) = 2(2|h|2) + (22|22).
\end{aligned}$$

exercise 2.18

类比于教材中将电子傀标在闭壳层结构下折半为电子对傀标，我也如此处理。此外，由于对闭壳层系统，同一能级上电子能量（不论其自旋）相同，即成立$\varepsilon_i = \varepsilon_{i'}$，从而求和范围折半后，和表达式的分母不变，从而在不改变结果的情况下，我将求和过程中出现的分母略去不写，以使过程简便，在最后结果中再加上它。那么，先分析求和范围变化，原求和裂为$2^4 = 16$组求和，而由求和表达式

exercise 2.19

exercise 2.20

exercise 2.21

exercise 2.22

exercise 2.23

exercise 2.24

exercise 2.25

exercise 2.26

exercise 2.27

exercise 2.28

exercise 2.29

exercise 2.30

exercise 2.31

EWFEW

Chapter 3 The Hartree-Fock Approximation

exercise 3.1

exercise 3.2

exercise 3.3

exercise 3.4

exercise 3.5

exercise 3.6

ESGRZBT

exercise 3.7

exercise 3.8

exercise 3.9

exercise 3.10

exercise 3.11

exercise 3.12

exercise 3.13

exercise 3.14

exercise 3.15

exercise 3.16

exercise 3.17

exercise 3.18

exercise 3.19

exercise 3.20

exercise 3.21

exercise 3.22

exercise 3.23

exercise 3.24

exercise 3.25

exercise 3.26

exercise 3.27

exercise 3.28

exercise 3.29

exercise 3.30

exercise 3.31

exercise 3.32

exercise 3.33

exercise 3.34

exercise 3.35

exercise 3.36

exercise 3.37

exercise 3.38

exercise 3.39

exercise 3.40

exercise 3.41

exercise 3.42

exercise 3.43

exercise 3.44

exercise 3.45

Chapter 4 Configuration Interaction

exercise 4.1

exercise 4.2

exercise 4.3

exercise 4.4

exercise 4.5

exercise 4.6

exercise 4.7

exercise 4.8

exercise 4.9

exercise 4.10

exercise 4.11

exercise 4.12

exercise 4.13

exercise 4.14

exercise 4.15

exercise 4.16

exercise 4.17

exercise 4.18

exercise 4.19

exercise 4.20

exercise 4.21

exercise 4.22