Exercises from *Modern Quantum Chemistry Introduction to Advanced Electronic Structure Theory* by Attila Szabo and Neil S. Ostlund

modern-quantum-chemistry.pdf

Exercise 1.1

Rewriting Equation (1.13) as

$$\mathrm{O}\vec{e}_j = \sum_{k=1}^{3} \vec{e_k} O_{kj}$$

Taking the dot product:

$$\vec{e_i} \cdot \mathrm{O}\vec{e_j} = \sum_{k=1}^{3} \vec{e_i} \cdot \vec{e_k} O_{kj} = \sum_{k=1}^{3} \delta_{ik}\, O_{kj} = O_{ij}$$

$$\mathrm{O}\vec{a} = \vec{b}$$

$$\mathrm{O}\vec{a} = \sum_{i=1}^{3} \mathrm{O}\, \vec{e_i} a_i = \sum_{i=1}^{3} b_i \vec{e_i}$$

$$\mathrm{O}a_i = \sum_{j=1}^{3} O_{ij} a_j = b_i$$

Exercise 1.2

$$A = \begin{pmatrix} 1 & 1 & 0 \\ 1 & 2 & 2 \\ 0 & 2 & -1 \end{pmatrix}, B = \begin{pmatrix} 1 & -1 & 1 \\ -1 & 0 & 0 \\ 1 & 0 & 1 \end{pmatrix}$$

$$C = \begin{pmatrix} 0 & -1 & 1 \\ 1 & -1 & 3 \\ -3 & 0 & -1 \end{pmatrix}$$

Verification by a homegrown computer program:

A * B = C

```
 0   -1    1
 1   -1    3
-3    0   -1
```

Exercise 1.2 page 5 Commutator

0	-2	4
2	0	3
-4	-3	0

Exercise 1.2 page 5 Anticommutator

0	0	-2
0	-2	3
-2	3	-2

[A, B] = AB - BA commutator Abelian [A, B] = 0
[A, BC] = ABC - BCA = ABC - BAC + BAC - BCA = [A, B]C + B[A, C]
[AB, C] = ABC - CAB = ABC - ACB + ACB - CAB = A[B, C] + [A, C]B
{A, B} = AB + BA anti-commutator
{A, BC} = ABC + BCA = ABC - BAC + BAC + BCA = [A, B]C + B{A, C}
{AB, C} = ABC + CAB = ABC - ACB + ACB + CAB = A[B, C] + {A, C}B

Exercise 1.3

Ac * Bc = Cc

-5 +	31i	-5 +	37i	-8 +	44i
4 +	68i	4 +	82i	1 +	97i
4 +	103i	4 +	128i	1 +	151i

Cc adjoint

-5 -	31i	4 -	68i	4 -	103i
-5 -	37i	4 -	82i	4 -	128i
-8 -	44i	1 -	97i	1 -	151i

Bc adjoint * Ac adjoint

-5 -	31i	4 -	68i	4 -	103i
-5 -	37i	4 -	82i	4 -	128i
-8 -	44i	1 -	97i	1 -	151i

Exercise 1.4

$$A = \begin{pmatrix} a & b \\ c & d \end{pmatrix}, B = \begin{pmatrix} e & f \\ g & i \end{pmatrix}, AB = \begin{pmatrix} ae + bg & af + bi \\ ce + dg & cf + di \end{pmatrix}, tr\ AB = ae + bg + cf + di$$

$$B = \begin{pmatrix} e & f \\ g & i \end{pmatrix}, A = \begin{pmatrix} a & b \\ c & d \end{pmatrix}, BA = \begin{pmatrix} ea + fc & eb + fd \\ ga + ic & gb + id \end{pmatrix}, tr\ BA = ea + fc + gb + id \therefore tr\ AB = tr\ BA\ since\ ab = ba \forall a, b \in \mathbb{R}$$

$$A = \begin{pmatrix} a & b \\ c & d \end{pmatrix}, A^{-1} = \frac{1}{ad - bc}\begin{pmatrix} d & -b \\ -c & a \end{pmatrix}$$

$$AA^{-1} = \frac{1}{ad-bc}\begin{pmatrix} a & b \\ c & d \end{pmatrix}\begin{pmatrix} d & -b \\ -c & a \end{pmatrix} = \frac{1}{ad-bc}\begin{pmatrix} ad-bc & -ab+ba \\ cd-dc & -cb+da \end{pmatrix}$$
$$= \frac{1}{ad-bc}\begin{pmatrix} ad-bc & 0 \\ 0 & -db+da \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = I, since\ ab = ba \forall a, b \in \mathbb{R}$$

Ar matrix

2	3	-1
4	4	-3
-2	3	-1

Ar Conte & de Boor inverse = 1

0.25	0	-0.25
0.5	-0.2	0.1
1	-0.6	-0.2

Ar * Ar inverse

1	0	0
0	1	0
0	0	1

Ac

```
+        1 +        1i  +        2 +        1i  +        3 +        2i
+        4 +        3i  +        5 +        0i  +        6 +        1i
+        7 +        0i  +        8 +        2i  +        9 +        4i
```

Ac inverse = 1

```
+0.0215285 +0.0247578i  -0.00538213 - 0.256189i +0.0365985 + 0.142088i
-  1.27879 + 0.329386i  + 0.319699 + 0.417653i  +  0.22605 - 0.240043i
+ 0.986006 - 0.466093i  - 0.246502 - 0.133477i  - 0.123789 + 0.107643i
```

Ac * AC inverse

```
+        1 -        0i  +        0 +        0i  +        0 -        0i
+        0 +        0i  +        1 +        0i  +        0 +        0i
-        0 -        0i  +        0 +        0i  +        1 -        0i
```