Modern Quantum Chemistry, Szabo & Ostlund
HW

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Contents

1 Mathematical Review

1.1 Linear Algebra

1.1.1 3-D Vector Algebra

Ex 1.1

a)

$$\mathscr{O}\mathbf{e}_j = \sum_{i=1}^{3} \mathbf{e}_i O_{ij} \tag{1.1}$$

$$\mathbf{e}_i \cdot \mathscr{O}\mathbf{e}_j = \mathbf{e}_i \cdot \sum_{i=1}^{3} \mathbf{e}_i O_{ij} = O_{ij} \tag{1.2}$$

b)

$$\begin{aligned} \mathbf{b} = \mathscr{O}\mathbf{a} &= \sum_{i=1}^{3} a_i \sum_{j=1}^{3} \mathbf{e}_j O_{ji} \\ &= \sum_{j=1}^{3} a_j \sum_{i=1}^{3} \mathbf{e}_i O_{ij} = \sum_{i=1}^{3} \mathbf{e}_i \sum_{j=1}^{3} a_j O_{ij} \end{aligned} \tag{1.3}$$

thus

$$\mathbf{b}_i = \sum_{j=1}^{3} a_j O_{ij} \tag{1.4}$$

Ex 1.2

$$[\mathbf{A}, \mathbf{B}] = \begin{bmatrix} 0 & -2 & 4 \\ 2 & 0 & 3 \\ -4 & -3 & 0 \end{bmatrix} \tag{1.5}$$

$$\{\mathbf{A}, \mathbf{B}\} = \begin{bmatrix} 0 & 0 & -2 \\ 0 & -2 & 3 \\ -2 & 3 & -2 \end{bmatrix} \tag{1.6}$$

1.1.2 Matrices

Ex 1.3

$$(AB)_{nk} = \sum_{m}^{M} A_{nm} B_{mk} \tag{1.7}$$

$$(AB)^\dagger_{kn} = (AB)^*_{nk} = \sum_{m}^{M} A^*_{nm} B^*_{mk} = \sum_{m}^{M} B^\dagger_{km} A^\dagger_{mn} = (B^\dagger A^\dagger)_{kn} \tag{1.8}$$

thus

$$(\mathbf{AB})^\dagger = \mathbf{B}^\dagger \mathbf{A}^\dagger \tag{1.9}$$

Ex 1.4

a. suppose $\mathbf{A}$ is $N \times M$ and $\mathbf{B}$ is $M \times N$

$$\operatorname{tr} \mathbf{AB} = \sum_{n}^{N} (AB)_{nn} = \sum_{n}^{N} \sum_{m}^{M} A_{nm} B_{mn} = \sum_{m}^{M} \sum_{n}^{N} B_{mn} A_{nm} = \sum_{m}^{M} (BA)_{mm} = \operatorname{tr} \mathbf{BA} \tag{1.10}$$

b.

$$\mathbf{AB}(\mathbf{AB})^{-1} = \mathbf{1} \tag{1.11}$$
$$\mathbf{B}^{-1}\mathbf{A}^{-1}\mathbf{AB}(\mathbf{AB})^{-1} = \mathbf{B}^{-1}\mathbf{A}^{-1}\mathbf{1} \tag{1.12}$$
$$\mathbf{B}^{-1}(\mathbf{A}^{-1}\mathbf{A})\mathbf{B}(\mathbf{AB})^{-1} = \mathbf{B}^{-1}\mathbf{A}^{-1} \tag{1.13}$$
$$\mathbf{B}^{-1}\mathbf{1}\mathbf{B}(\mathbf{AB})^{-1} = \mathbf{B}^{-1}\mathbf{A}^{-1} \tag{1.14}$$

thus

$$(\mathbf{AB})^{-1} = \mathbf{B}^{-1}\mathbf{A}^{-1} \tag{1.15}$$

c.

$$\mathbf{B} = \mathbf{U}^\dagger\mathbf{AU} \tag{1.16}$$

huhhj

$$\mathbf{UBU}^\dagger = \mathbf{UU}^\dagger\mathbf{AUU}^\dagger = \mathbf{1A1} = \mathbf{A} \tag{1.17}$$

d. $\because$ $\mathbf{C}$ is Hermitian, $\therefore$

$$\mathbf{C} = \mathbf{C}^\dagger \tag{1.18}$$
$$\mathbf{AB} = (\mathbf{AB})^\dagger = \mathbf{B}^\dagger\mathbf{A}^\dagger \tag{1.19}$$

Since $\mathbf{A}$, $\mathbf{B}$ are Hermitian,

$$\mathbf{AB} = \mathbf{B}^\dagger\mathbf{A}^\dagger = \mathbf{BA} \tag{1.20}$$

$\therefore$

$$[\mathbf{A}, \mathbf{B}] = \mathbf{AB} - \mathbf{BA} = 0 \tag{1.21}$$

i.e. $\mathbf{A}$, $\mathbf{B}$ commute

e. Since $\mathbf{A}$ is Hermitian,

$$\mathbf{A} = \mathbf{A}^\dagger \tag{1.22}$$

thus

$$(\mathbf{A}^{1-})^\dagger\mathbf{A} = (\mathbf{A}^{1-})^\dagger\mathbf{A}^\dagger = (\mathbf{AA}^{-1})^\dagger = \mathbf{1}^\dagger = \mathbf{1} \tag{1.23}$$

thus

$$(\mathbf{A}^{1-})^\dagger\mathbf{AA}^{-1} = \mathbf{A}^{-1} \tag{1.24}$$
$$(\mathbf{A}^{1-})^\dagger = \mathbf{A}^{-1} \tag{1.25}$$

i.e. $\mathbf{A}^{-1}$, if it exists, is Hermitian.

f. Suppose

$$\mathbf{A}^{-1} = \begin{pmatrix} x & y \\ z & w \end{pmatrix} \tag{1.26}$$

thus

$$\begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix}\begin{pmatrix} x & y \\ z & w \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \tag{1.27}$$

the solution is

$$\begin{aligned} x &= \frac{A_{22}}{A_{11}A_{22} - A_{12}A_{21}} \\ y &= \frac{-A_{12}}{A_{11}A_{22} - A_{12}A_{21}} \\ z &= \frac{-A_{21}}{A_{11}A_{22} - A_{12}A_{21}} \\ w &= \frac{A_{11}}{A_{11}A_{22} - A_{12}A_{21}} \end{aligned} \tag{1.28}$$

thus

$$\mathbf{A}^{-1} = \frac{1}{\det(\mathbf{A})}\begin{pmatrix} A_{22} & -A_{12} \\ -A_{21} & A_{11} \end{pmatrix} \tag{1.29}$$