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

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

Ex 1.5 Suppose

$$\mathbf{A} = \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix} \tag{1.30}$$

1.

$$\begin{vmatrix} 0 & 0 \\ A_{21} & A_{22} \end{vmatrix} = 0 \cdot A_{22} - 0 \cdot A_{21} = 0 \tag{1.31}$$

$$\begin{vmatrix} 0 & A_{12} \\ 0 & A_{22} \end{vmatrix} = 0 \cdot A_{22} - 0 \cdot A_{12} = 0 \tag{1.32}$$

2.

$$\det(\mathbf{A}) = A_{11}A_{22} - 0 \cdot 0 = A_{11}A_{22} \tag{1.33}$$

3.

$$\det(\mathbf{A}) = A_{11}A_{22} - A_{12}A_{21} \tag{1.34}$$

$$\begin{vmatrix} A_{21} & A_{22} \\ A_{11} & A_{12} \end{vmatrix} = A_{21}A_{12} - A_{22}A_{11} = -\det(\mathbf{A}) \tag{1.35}$$

4.

$$\det\left(\mathbf{A}^\dagger\right)^* = \begin{vmatrix} A_{11}^* & A_{21}^* \\ A_{12}^* & A_{22}^* \end{vmatrix}^* = (A_{11}^* A_{22}^* - A_{21}^* A_{12}^*)^* = A_{11}A_{22} - A_{12}A_{21} = \det(\mathbf{A}) \tag{1.36}$$

5. Suppose $\mathbf{B} = \begin{pmatrix} B_{11} & B_{12} \\ B_{21} & B_{22} \end{pmatrix}$

$$\begin{aligned} \det(\mathbf{AB}) &= \begin{vmatrix} A_{11}B_{11} + A_{12}B_{21} & A_{11}B_{12} + A_{12}B_{22} \\ A_{21}B_{11} + A_{22}B_{21} & A_{21}B_{12} + A_{22}B_{22} \end{vmatrix} \\ &= (A_{11}B_{11} + A_{12}B_{21})(A_{21}B_{12} + A_{22}B_{22}) - (A_{11}B_{12} + A_{12}B_{22})(A_{21}B_{11} + A_{22}B_{21}) \\ &= A_{11}B_{11}A_{21}B_{12} + A_{11}B_{11}A_{22}B_{22} + A_{12}B_{21}A_{21}B_{12} + A_{12}B_{21}A_{22}B_{22} \\ &\quad - (A_{11}B_{12}A_{21}B_{11} + A_{11}B_{12}A_{22}B_{21} + A_{12}B_{22}A_{21}B_{11} + A_{12}B_{22}A_{22}B_{21}) \\ &= A_{11}B_{11}A_{22}B_{22} + A_{12}B_{21}A_{21}B_{12} - A_{11}B_{12}A_{22}B_{21} - A_{12}B_{22}A_{21}B_{11} \end{aligned} \tag{1.37}$$

$$\begin{aligned} \det(\mathbf{A})\det(\mathbf{B}) &= (A_{11}A_{22} - A_{12}A_{21})(B_{11}B_{22} - B_{12}B_{21}) \\ &= A_{11}A_{22}B_{11}B_{22} - A_{11}A_{22}B_{12}B_{21} - A_{12}A_{21}B_{11}B_{22} + A_{12}A_{21}B_{12}B_{21} \\ &= A_{11}B_{11}A_{22}B_{22} + A_{12}B_{21}A_{21}B_{12} - A_{11}B_{12}A_{22}B_{21} - A_{12}B_{22}A_{21}B_{11} \end{aligned} \tag{1.38}$$

$\therefore$

$$\det(\mathbf{A})\det(\mathbf{B}) = \det(\mathbf{AB}) \tag{1.39}$$

Ex 1.6

6. If two rows (e.g. ith and jth) are equal

$$\det(\mathbf{A}) = \begin{vmatrix} & \cdots & \cdots & \\ A_{i1} & A_{i2} & \cdots & A_{in} \\ & \cdots & \cdots & \\ A_{j1} & A_{j2} & \cdots & A_{jn} \\ & \cdots & \cdots & \end{vmatrix} \overset{1.5.3}{=\!=} - \begin{vmatrix} & \cdots & \cdots & \\ A_{j1} & A_{j2} & \cdots & A_{jn} \\ & \cdots & \cdots & \\ A_{i1} & A_{i2} & \cdots & A_{in} \\ & \cdots & \cdots & \end{vmatrix} = - \begin{vmatrix} & \cdots & \cdots & \\ A_{i1} & A_{i2} & \cdots & A_{in} \\ & \cdots & \cdots & \\ A_{j1} & A_{j2} & \cdots & A_{jn} \\ & \cdots & \cdots & \end{vmatrix} \tag{1.40}$$

i.e.

$$\det(\mathbf{A}) = -\det(\mathbf{A}) \tag{1.41}$$

thus

$$\det(\mathbf{A}) = 0 \tag{1.42}$$

7. From Ex 1.5.5, we have

$$\det(\mathbf{A})\det\left(\mathbf{A}^{-1}\right) = \det(\mathbf{1}) = 1 \tag{1.43}$$

thus

$$\det\left(\mathbf{A}^{-1}\right) = \det(\mathbf{A})^{-1} \tag{1.44}$$