Modern Quantum Chemistry, Szabo & Ostlund
HW

王石嵘

August 10, 2019

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.

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

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