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)

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

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

b)

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

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.