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)

$$\mathcal{O}\mathbf{e}_j = \sum_{i=1}^{3} \mathbf{e}_i O_{ij} \tag{1.1.1}$$

$$\mathbf{e}_i \cdot \mathcal{O}\mathbf{e}_j = \mathbf{e}_i \cdot \sum_{i=1}^{3} \mathbf{e}_i O_{ij} = O_{ij} \tag{1.1.2}$$

b)

$$\begin{aligned} \mathbf{b} = \mathcal{O}\mathbf{a} &= \sum_{i=1}^{3} a_i \sum_{j=1}^{3} \mathbf{e}_j O_{ji} \\ &= \sum_{j=1}^{3} a_j \sum_{i=1}^{3} \mathbf{e}_i O_{ij} = \sum_{i=1}^{3} \mathbf{e}_i \sum_{j=1}^{3} a_j O_{ij} \end{aligned} \tag{1.1.3}$$

thus

$$\mathbf{b}_i = \sum_{j=1}^{3} a_j O_{ij} \tag{1.1.4}$$

Ex 1.2

$$[\mathbf{A}, \mathbf{B}] = \begin{bmatrix} 0 & -2 & 4 \\ 2 & 0 & 3 \\ -4 & -3 & 0 \end{bmatrix} \tag{1.1.5}$$

$$\{\mathbf{A}, \mathbf{B}\} = \begin{bmatrix} 0 & 0 & -2 \\ 0 & -2 & 3 \\ -2 & 3 & -2 \end{bmatrix} \tag{1.1.6}$$

1.1.2 Matrices

Ex 1.3

$$(AB)_{nk} = \sum_{m}^{M} A_{nm} B_{mk} \tag{1.1.7}$$

$$(AB)^{\dagger}_{kn} = (AB)^{*}_{nk} = \sum_{m}^{M} A^{*}_{nm} B^{*}_{mk} = \sum_{m}^{M} B^{\dagger}_{km} A^{\dagger}_{mn} = (B^{\dagger} A^{\dagger})_{kn} \tag{1.1.8}$$

thus

$$(\mathbf{AB})^{\dagger} = \mathbf{B}^{\dagger} \mathbf{A}^{\dagger} \tag{1.1.9}$$

Ex 1.4

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

$$\operatorname{tr} \mathbf{AB} = \sum_{n}^{N} (AB)_{nn} = \sum_{n}^{N} \sum_{m}^{M} A_{nm} B_{mn} = \sum_{m}^{M} \sum_{n}^{N} B_{mn} A_{nm} = \sum_{m}^{M} (BA)_{mm} = \operatorname{tr} \mathbf{BA} \tag{1.1.10}$$

b.

$$\mathbf{AB}(\mathbf{AB})^{-1} = \mathbf{1} \tag{1.1.11}$$
$$\mathbf{B}^{-1}\mathbf{A}^{-1}\mathbf{AB}(\mathbf{AB})^{-1} = \mathbf{B}^{-1}\mathbf{A}^{-1}\mathbf{1} \tag{1.1.12}$$
$$\mathbf{B}^{-1}(\mathbf{A}^{-1}\mathbf{A})\mathbf{B}(\mathbf{AB})^{-1} = \mathbf{B}^{-1}\mathbf{A}^{-1} \tag{1.1.13}$$
$$\mathbf{B}^{-1}\mathbf{1}\mathbf{B}(\mathbf{AB})^{-1} = \mathbf{B}^{-1}\mathbf{A}^{-1} \tag{1.1.14}$$

thus

$$(\mathbf{AB})^{-1} = \mathbf{B}^{-1}\mathbf{A}^{-1} \tag{1.1.15}$$

c.

$$\mathbf{B} = \mathbf{U}^{\dagger}\mathbf{AU} \tag{1.1.16}$$

huhhj

$$\mathbf{UBU}^{\dagger} = \mathbf{UU}^{\dagger}\mathbf{AUU}^{\dagger} = \mathbf{1A1} = \mathbf{A} \tag{1.1.17}$$

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

$$\mathbf{C} = \mathbf{C}^{\dagger} \tag{1.1.18}$$
$$\mathbf{AB} = (\mathbf{AB})^{\dagger} = \mathbf{B}^{\dagger}\mathbf{A}^{\dagger} \tag{1.1.19}$$

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

$$\mathbf{AB} = \mathbf{B}^{\dagger}\mathbf{A}^{\dagger} = \mathbf{BA} \tag{1.1.20}$$

$\therefore$

$$[\mathbf{A}, \mathbf{B}] = \mathbf{AB} - \mathbf{BA} = 0 \tag{1.1.21}$$

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

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

$$\mathbf{A} = \mathbf{A}^{\dagger} \tag{1.1.22}$$

thus

$$(\mathbf{A}^{1-})^{\dagger}\mathbf{A} = (\mathbf{A}^{1-})^{\dagger}\mathbf{A}^{\dagger} = (\mathbf{AA}^{-1})^{\dagger} = \mathbf{1}^{\dagger} = \mathbf{1} \tag{1.1.23}$$

thus

$$(\mathbf{A}^{1-})^{\dagger}\mathbf{AA}^{-1} = \mathbf{A}^{-1} \tag{1.1.24}$$
$$(\mathbf{A}^{1-})^{\dagger} = \mathbf{A}^{-1} \tag{1.1.25}$$

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

f. Suppose

$$\mathbf{A}^{-1} = \begin{pmatrix} x & y \\ z & w \end{pmatrix} \tag{1.1.26}$$

thus

$$\begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix}\begin{pmatrix} x & y \\ z & w \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \tag{1.1.27}$$

the solution is

$$\begin{aligned} x &= \frac{A_{22}}{A_{11}A_{22} - A_{12}A_{21}} \\ y &= \frac{-A_{12}}{A_{11}A_{22} - A_{12}A_{21}} \\ z &= \frac{-A_{21}}{A_{11}A_{22} - A_{12}A_{21}} \\ w &= \frac{A_{11}}{A_{11}A_{22} - A_{12}A_{21}} \end{aligned} \tag{1.1.28}$$

thus

$$\mathbf{A}^{-1} = \frac{1}{\det(\mathbf{A})}\begin{pmatrix} A_{22} & -A_{12} \\ -A_{21} & A_{11} \end{pmatrix} \tag{1.1.29}$$

1.1.3 Determinants

Ex 1.5 Suppose

$$\mathbf{A} = \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix} \tag{1.1.30}$$

1.

$$\begin{vmatrix} 0 & 0 \\ A_{21} & A_{22} \end{vmatrix} = 0 \cdot A_{22} - 0 \cdot A_{21} = 0 \tag{1.1.31}$$

$$\begin{vmatrix} 0 & A_{12} \\ 0 & A_{22} \end{vmatrix} = 0 \cdot A_{22} - 0 \cdot A_{12} = 0 \tag{1.1.32}$$

2.

$$\det(\mathbf{A}) = A_{11}A_{22} - 0 \cdot 0 = A_{11}A_{22} \tag{1.1.33}$$

3.

$$\det(\mathbf{A}) = A_{11}A_{22} - A_{12}A_{21} \tag{1.1.34}$$

$$\begin{vmatrix} A_{21} & A_{22} \\ A_{11} & A_{12} \end{vmatrix} = A_{21}A_{12} - A_{22}A_{11} = -\det(\mathbf{A}) \tag{1.1.35}$$

4.

$$\det\left(\mathbf{A}^\dagger\right)^* = \begin{vmatrix} A_{11}^* & A_{21}^* \\ A_{12}^* & A_{22}^* \end{vmatrix}^* = (A_{11}^*A_{22}^* - A_{21}^*A_{12}^*)^* = A_{11}A_{22} - A_{12}A_{21} = \det(\mathbf{A}) \tag{1.1.36}$$

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

$$\begin{aligned} \det(\mathbf{AB}) &= \begin{vmatrix} A_{11}B_{11} + A_{12}B_{21} & A_{11}B_{12} + A_{12}B_{22} \\ A_{21}B_{11} + A_{22}B_{21} & A_{21}B_{12} + A_{22}B_{22} \end{vmatrix} \\ &= (A_{11}B_{11} + A_{12}B_{21})(A_{21}B_{12} + A_{22}B_{22}) - (A_{11}B_{12} + A_{12}B_{22})(A_{21}B_{11} + A_{22}B_{21}) \\ &= A_{11}B_{11}A_{21}B_{12} + A_{11}B_{11}A_{22}B_{22} + A_{12}B_{21}A_{21}B_{12} + A_{12}B_{21}A_{22}B_{22} \\ &\quad - (A_{11}B_{12}A_{21}B_{11} + A_{11}B_{12}A_{22}B_{21} + A_{12}B_{22}A_{21}B_{11} + A_{12}B_{22}A_{22}B_{21}) \\ &= A_{11}B_{11}A_{22}B_{22} + A_{12}B_{21}A_{21}B_{12} - A_{11}B_{12}A_{22}B_{21} - A_{12}B_{22}A_{21}B_{11} \end{aligned} \tag{1.1.37}$$

$$\begin{aligned} \det(\mathbf{A})\det(\mathbf{B}) &= (A_{11}A_{22} - A_{12}A_{21})(B_{11}B_{22} - B_{12}B_{21}) \\ &= A_{11}A_{22}B_{11}B_{22} - A_{11}A_{22}B_{12}B_{21} - A_{12}A_{21}B_{11}B_{22} + A_{12}A_{21}B_{12}B_{21} \\ &= A_{11}B_{11}A_{22}B_{22} + A_{12}B_{21}A_{21}B_{12} - A_{11}B_{12}A_{22}B_{21} - A_{12}B_{22}A_{21}B_{11} \end{aligned} \tag{1.1.38}$$

$\therefore$

$$\det(\mathbf{A})\det(\mathbf{B}) = \det(\mathbf{AB}) \tag{1.1.39}$$

Ex 1.6

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

$$\det(\mathbf{A}) = \begin{vmatrix} & \dots & \dots & \\ A_{i1} & A_{i2} & \dots & A_{in} \\ & \dots & \dots & \\ A_{j1} & A_{j2} & \dots & A_{jn} \\ & \dots & \dots & \end{vmatrix} \overset{1.5.3}{=\!=} -\begin{vmatrix} & \dots & \dots & \\ A_{j1} & A_{j2} & \dots & A_{jn} \\ & \dots & \dots & \\ A_{i1} & A_{i2} & \dots & A_{in} \\ & \dots & \dots & \end{vmatrix} = -\begin{vmatrix} & \dots & \dots & \\ A_{i1} & A_{i2} & \dots & A_{in} \\ & \dots & \dots & \\ A_{j1} & A_{j2} & \dots & A_{jn} \\ & \dots & \dots & \end{vmatrix} \tag{1.1.40}$$

i.e.

$$\det(\mathbf{A}) = -\det(\mathbf{A}) \tag{1.1.41}$$

thus

$$\det(\mathbf{A}) = 0 \tag{1.1.42}$$

7. From Ex 1.5.5, we have

$$\det(\mathbf{A})\det\left(\mathbf{A}^{-1}\right) = \det(\mathbf{1}) = 1 \tag{1.1.43}$$

thus

$$\det\left(\mathbf{A}^{-1}\right) = \det(\mathbf{A})^{-1} \tag{1.1.44}$$

8.

$$\mathbf{A}\mathbf{A}^{\dagger} = \mathbf{1} \Rightarrow \det(\mathbf{A})\det\left(\mathbf{A}^{\dagger}\right) = \det(\mathbf{1}) = 1 \tag{1.1.45}$$

From Ex 1.5.4, we have

$$\det(\mathbf{A})\det(\mathbf{A})^* = 1 \tag{1.1.46}$$

9. From Ex 1.5.5, we get

$$\det\left(\mathbf{U}^{\dagger}\right)\det(\mathbf{O})\det(\mathbf{U}) = \det(\mathbf{\Omega}) \tag{1.1.47}$$

and

$$\det\left(\mathbf{U}^{\dagger}\right)\det(\mathbf{U}) = \det(\mathbf{1}) = 1 \tag{1.1.48}$$

$\therefore$

$$\det(\mathbf{O}) = \det(\mathbf{\Omega}) \tag{1.1.49}$$

Ex 1.7 If $\det(\mathbf{A}) \neq 0$, thus $\mathbf{A}^{-1}$ exists, we have

$$\mathbf{A}^{-1}\mathbf{A}\mathbf{c} = \mathbf{0} \Rightarrow \mathbf{c} = \mathbf{0} \tag{1.1.50}$$

□

1.1.4 N-D Complex Vector Spaces

1.1.5 Change of Basis

Ex 1.8

$$\Omega_{\alpha\beta} = \sum_{ij} U^{\dagger}_{\alpha i} O_{ij} U_{j\beta} \tag{1.1.51}$$

gives

$$\begin{aligned} \operatorname{tr}\mathbf{\Omega} &= \sum_{\alpha}\Omega_{\alpha\alpha} = \sum_{\alpha}\sum_{ij} U^{\dagger}_{\alpha i} O_{ij} U_{j\alpha} \\ &= \sum_{ij} O_{ij}\sum_{\alpha} U_{j\alpha}U^{\dagger}_{\alpha i} = \sum_{ij} O_{ij}\delta_{ji} = \operatorname{tr}\mathbf{O} \end{aligned} \tag{1.1.52}$$

1.1.6 The Eigenvalue Problem

Ex 1.9

$$\mathbf{O}\mathbf{U} = \mathbf{U}\boldsymbol{\omega} \Rightarrow \mathbf{O}\begin{pmatrix}\mathbf{c}^1 & \mathbf{c}^2 & \cdots & \mathbf{c}^N\end{pmatrix} = \begin{pmatrix}\omega_1\mathbf{c}_1 & \omega_2\mathbf{c}_2 & \cdots & \omega_N\mathbf{c}_N\end{pmatrix} \tag{1.1.53}$$

thus

$$\mathbf{O}\mathbf{c}^{\alpha} = \omega_{\alpha}\mathbf{c}^{\alpha} \tag{1.1.54}$$

Ex 1.10

$$\begin{cases} O_{11} - \omega + O_{12}c = 0 \\ O_{21} + (O_{22} - \omega)c = 0 \end{cases} \tag{1.1.55}$$

$$(O_{11} - \omega)(O_{22} - \omega) - O_{21}O_{12} = 0 \tag{1.1.56}$$

$$\omega^2 - (O_{11} + O_{22})\omega + O_{11}O_{22} - O_{21}O_{12} = 0 \tag{1.1.57}$$

$$\begin{cases} \omega_1 = \dfrac{1}{2}\left(O_{11} + O_{22} - \sqrt{(O_{11} - O_{22})^2 + 4O_{21}O_{12}}\right) \\ \omega_2 = \dfrac{1}{2}\left(O_{11} + O_{22} + \sqrt{(O_{11} - O_{22})^2 + 4O_{21}O_{12}}\right) \end{cases} \tag{1.1.58}$$

Ex 1.11

a)

$$\begin{vmatrix} 3-\omega & 1 \\ 1 & 3-\omega \end{vmatrix} = 0 \Rightarrow (3-\omega)^2 - 1 = 0 \tag{1.1.59}$$

Eigenvalues

$$\omega_1 = 2 \quad \omega_2 = 4 \tag{1.1.60}$$

Eigenvectors

$$\mathbf{c}^1 = \begin{pmatrix} 1 \\ -1 \end{pmatrix} \quad \mathbf{c}^2 = \begin{pmatrix} 1 \\ 1 \end{pmatrix} \tag{1.1.61}$$

$$\begin{vmatrix} 3-\omega & 1 \\ 1 & 2-\omega \end{vmatrix} = 0 \Rightarrow (3-\omega)(2-\omega) - 1 = 0 \tag{1.1.62}$$

Eigenvalues

$$\omega_1 = \frac{5+\sqrt{5}}{2} \quad \omega_2 = \frac{5-\sqrt{5}}{2} \tag{1.1.63}$$

Eigenvectors

$$\mathbf{c}^1 = \begin{pmatrix} \frac{1}{2}(1+\sqrt{5}) \\ 1 \end{pmatrix} \quad \mathbf{c}^2 = \begin{pmatrix} \frac{1}{2}(1-\sqrt{5}) \\ 1 \end{pmatrix} \tag{1.1.64}$$

b)

$$\theta_0 = \frac{1}{2}\tan^{-1}\frac{2O_{12}}{O_{11}-O_{12}} \tag{1.1.65}$$

for $\mathbf{A}$

$$\theta_0 = \frac{1}{2}\tan^{-1}\frac{2\times 1}{3-3} = \frac{\pi}{4} \tag{1.1.66}$$

Eigenvalues

$$\omega_1 = 2 \quad \omega_2 = 4 \tag{1.1.67}$$

Eigenvectors

$$\mathbf{c}^1 = \begin{pmatrix} \sqrt{2}/2 \\ -\sqrt{2}/2 \end{pmatrix} \quad \mathbf{c}^2 = \begin{pmatrix} \sqrt{2}/2 \\ \sqrt{2}/2 \end{pmatrix} \tag{1.1.68}$$

for $\mathbf{B}$

$$\theta_0 = \frac{1}{2}\tan^{-1}\frac{2\times 1}{3-2} = \frac{1}{2}\tan^{-1} 2 \tag{1.1.69}$$

Eigenvalues

$$\omega_1 = \frac{10}{5+\sqrt{5}} = \frac{5-\sqrt{5}}{2} \quad \omega_2 = \frac{10}{5-\sqrt{5}} = \frac{5+\sqrt{5}}{2} \tag{1.1.70}$$

Eigenvectors

$$\mathbf{c}^1 = \begin{pmatrix} \sqrt{\frac{\sqrt{5}+5}{10}} \\ \sqrt{\frac{2}{\sqrt{5}+5}} \end{pmatrix} = \sqrt{\frac{2}{\sqrt{5}+5}} \begin{pmatrix} \frac{1+\sqrt{5}}{2} \\ 1 \end{pmatrix} \tag{1.1.71}$$

$$\mathbf{c}^2 = \begin{pmatrix} \sqrt{\frac{2}{\sqrt{5}+5}} \\ -\sqrt{\frac{\sqrt{5}+5}{10}} \end{pmatrix} = -\sqrt{\frac{\sqrt{5}+5}{10}} \begin{pmatrix} \frac{1-\sqrt{5}}{2} \\ 1 \end{pmatrix} \tag{1.1.72}$$

Details are in `chap1-1.nb`

1.1.7 Functions of Matrices

Ex 1.12

a.

$$\mathbf{A}^n = \mathbf{U}\mathbf{a}^n\mathbf{U}^\dagger \tag{1.1.73}$$

$$\det(\mathbf{A}^n) = \det(\mathbf{U})\det(\mathbf{a}^n)\det\big(\mathbf{U}^\dagger\big) = \det(\mathbf{U})\det\big(\mathbf{U}^\dagger\big)\begin{vmatrix} a_1^n & & & \\ & a_2^n & & \\ & & \ddots & \\ & & & a_N^n \end{vmatrix} = a_1^n a_2^n \cdots a_N^n \tag{1.1.74}$$

b. From 1.4.a, we have

$$\operatorname{tr}\mathbf{A}^n = \operatorname{tr}\big(\mathbf{U}\mathbf{a}^n\mathbf{U}^\dagger\big) = \operatorname{tr}\big(\mathbf{U}\mathbf{U}^\dagger\mathbf{a}^n\big) = \operatorname{tr}(\mathbf{a}^n) = \sum_{\alpha=1}^{N} a_\alpha^n \tag{1.1.75}$$

c.

$$\mathbf{U}^\dagger(\omega\mathbf{1} - \mathbf{A})\mathbf{U} = \omega\mathbf{1} - \mathbf{a} \tag{1.1.76}$$

$$(\omega\mathbf{1} - \mathbf{A})^{-1} = [(\mathbf{U}(\omega\mathbf{1} - \mathbf{a})\mathbf{U}^\dagger]^{-1} = \mathbf{U}(\omega\mathbf{1} - \mathbf{a})^{-1}\mathbf{U}^\dagger \tag{1.1.77}$$

while

$$(\omega\mathbf{1} - \mathbf{a})^{-1} = \begin{pmatrix} \omega - a_1 & & & \\ & \omega - a_2 & & \\ & & \ddots & \\ & & & \omega - a_N \end{pmatrix}^{-1} = \begin{pmatrix} \frac{1}{\omega - a_1} & & & \\ & \frac{1}{\omega - a_2} & & \\ & & \ddots & \\ & & & \frac{1}{\omega - a_N} \end{pmatrix} \tag{1.1.78}$$

thus

$$\mathbf{G}(\omega) = (\omega\mathbf{1} - \mathbf{A})^{-1} = \mathbf{U}\begin{pmatrix} \frac{1}{\omega - a_1} & & & \\ & \frac{1}{\omega - a_2} & & \\ & & \ddots & \\ & & & \frac{1}{\omega - a_N} \end{pmatrix}\mathbf{U}^\dagger \tag{1.1.79}$$

$$\mathbf{G}(\omega)_{ij} = \sum_\alpha U_{i\alpha}\frac{1}{\omega - a_\alpha}U^\dagger_{\alpha j} = \sum_\alpha \frac{U_{i\alpha}U^*_{j\alpha}}{\omega - a_\alpha} \tag{1.1.80}$$

Since $U_{i\alpha} = \langle i \,|\, \alpha\rangle$, $U^\dagger_{\alpha j} = U^*_{j\alpha} = \langle \alpha \,|\, j\rangle$

$$\mathbf{G}(\omega)_{ij} = \sum_\alpha \frac{\langle i \,|\, \alpha\rangle\,\langle \alpha \,|\, j\rangle}{\omega - a_\alpha} \tag{1.1.81}$$

Ex 1.13 The eigenvalues and eigenvectors of $\mathbf{A}$ are

$$\omega_1 = a - b \quad \omega_2 = a + b \tag{1.1.82}$$

$$\mathbf{c}^1 = \begin{pmatrix} 1 \\ -1 \end{pmatrix} \quad \mathbf{c}^2 = \begin{pmatrix} 1 \\ 1 \end{pmatrix} \tag{1.1.83}$$

$$\mathbf{A} = \mathbf{U}\mathbf{a}\mathbf{U}^\dagger = \frac{\sqrt{2}}{2}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}\begin{pmatrix} a+b & 0 \\ 0 & a-b \end{pmatrix}\frac{\sqrt{2}}{2}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \tag{1.1.84}$$

$$\begin{aligned} f(\mathbf{A}) = \mathbf{U}f(\mathbf{a})\mathbf{U}^\dagger &= \frac{1}{2}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}\begin{pmatrix} f(a+b) & 0 \\ 0 & f(a-b) \end{pmatrix}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \\ &= \frac{1}{2}\begin{pmatrix} f(a+b) & f(a-b) \\ f(a+b) & -f(a-b) \end{pmatrix}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \\ &= \frac{1}{2}\begin{pmatrix} f(a+b) + f(a-b) & f(a+b) - f(a-b) \\ f(a+b) - f(a-b) & f(a+b) + f(a-b) \end{pmatrix} \end{aligned} \tag{1.1.85}$$

1.2 Orthogonal Functions, Eigenfunctions, and Operators

Ex 1.14

$$\int_{-\infty}^{\infty} \mathrm{d}x a(x)\delta(x) = \lim_{\varepsilon \to 0} \int_{-\varepsilon}^{\varepsilon} \mathrm{d}x a(x) \frac{1}{2\varepsilon} = \lim_{\varepsilon \to 0} \frac{1}{2\varepsilon} \int_{-\varepsilon}^{\varepsilon} \mathrm{d}x a(x) \xlongequal{\text{L'Hôpital}} \lim_{\varepsilon \to 0} \frac{a(\varepsilon) - [-a(-\varepsilon)]}{2} = a(0) \tag{1.2.1}$$

Ex 1.15

$$\begin{aligned}\int \mathrm{d}x \psi_j^*(x) \mathcal{O} \psi_i(x) &= \int \mathrm{d}x \psi_j^*(x) \sum_k \psi_k(x) O_{ki} = \sum_k O_{ki} \int \mathrm{d}x \psi_j^*(x) \psi_k(x) \\ &= \sum_k O_{ki} \delta_{jk} = O_{ji}\end{aligned} \tag{1.2.2}$$

In bra-ket notation, (1) becomes

$$\mathcal{O} \left| i \right\rangle = \sum_j \left| j \right\rangle \left\langle j \,|\, \mathcal{O} \,|\, i \right\rangle \tag{1.2.3}$$

which is identical to Eq.(1.55) in the textbook.

Ex 1.16 With bra-ket notation,

$$\mathcal{O} \sum_{\mathrm{i}=1}^{\infty} c_i \left| i \right\rangle = \omega \sum_{\mathrm{i}=1}^{\infty} c_i \left| i \right\rangle \tag{1.2.4}$$

Multiply by $\langle j |$

$$\sum_{\mathrm{i}=1}^{\infty} c_i \left\langle j \,|\, \mathcal{O} \,|\, i \right\rangle = \omega \sum_{\mathrm{i}=1}^{\infty} c_i \left\langle j \,|\, i \right\rangle = \omega c_j \tag{1.2.5}$$

i.e.

$$\sum_{\mathrm{i}=1}^{\infty} O_{ji} c_i = \omega c_j \tag{1.2.6}$$

$$\mathbf{O}\mathbf{c} = \omega \mathbf{c} \tag{1.2.7}$$

It's similar to prove that without bra-ket notation.

Ex 1.17

a.

$$\int \mathrm{d}x \left\langle i | x \right| \left\langle x \,|\, j \right\rangle = \left\langle i \,|\, j \right\rangle = \delta_{ij} \tag{1.2.8}$$

i.e.

$$\int \mathrm{d}x \psi_i^*(x) \Psi_j(x) = \delta_{ij} \tag{1.2.9}$$

b.

$$\sum_{\mathrm{i}=1}^{\infty} \left\langle x \,|\, i \right\rangle \left\langle i \,|\, x' \right\rangle = \left\langle x \,|\, x' \right\rangle = \delta(x - x') \tag{1.2.10}$$

thus

$$\sum_{\mathrm{i}=1}^{\infty} \psi_i^*(x) \psi_i(x') = \sum_{\mathrm{i}=1}^{\infty} \left\langle x \,|\, i \right\rangle \left\langle i \,|\, x' \right\rangle = \delta(x - x') \tag{1.2.11}$$

c.

1.2.1