Modern Quantum Chemistry, Szabo & Ostlund
HW

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Contents

2 Many-electron Wave Functions and Operators

2.1 The Electronic Problem

2.1.1 Atomic Units

2.1.2 The B-O Approximation

2.1.3 The Antisymmetry or Pauli Exclusion Principle

2.2 Orbitals, Slater Determinants, and Basis Functions

2.2.1 Spin Orbitals and Spatial Orbitals

Ex 2.1 Consider $\langle \chi_k \,|\, \chi_m \rangle$. If $k = m$,

$$\langle \chi_{2i-1} \,|\, \chi_{2i-1} \rangle = \langle \psi_i^\alpha \,|\, \psi_i^\alpha \rangle \langle \alpha \,|\, \alpha \rangle = 1 \tag{2.2.1}$$

$$\langle \chi_{2i} \,|\, \chi_{2i} \rangle = \left\langle \psi_i^\beta \,\middle|\, \psi_i^\beta \right\rangle \langle \alpha \,|\, \alpha \rangle = 1 \tag{2.2.2}$$

thus

$$\langle \chi_k \,|\, \chi_k \rangle = 1 \tag{2.2.3}$$

If $k \neq m$, three cases may occur as below

$$\langle \chi_{2i-1} \,|\, \chi_{2j-1} \rangle = \left\langle \psi_i^\alpha \,\middle|\, \psi_j^\alpha \right\rangle \langle \alpha \,|\, \alpha \rangle = 0 \cdot 1 = 0 \qquad (i \neq j) \tag{2.2.4}$$

$$\langle \chi_{2i-1} \,|\, \chi_{2j} \rangle = \left\langle \psi_i^\alpha \,\middle|\, \psi_j^\beta \right\rangle \langle \alpha \,|\, \beta \rangle = S_{ij} \cdot 0 = 0 \tag{2.2.5}$$

$$\langle \chi_{2i} \,|\, \chi_{2j} \rangle = \left\langle \psi_i^\beta \,\middle|\, \psi_j^\beta \right\rangle \langle \beta \,|\, \beta \rangle = 0 \cdot 1 = 0 \qquad (i \neq j) \tag{2.2.6}$$

thus

$$\langle \chi_k \,|\, \chi_m \rangle = 0 \qquad (k \neq m) \tag{2.2.7}$$

Overall,

$$\langle \chi_k \,|\, \chi_m \rangle = \delta_{km} \tag{2.2.8}$$

2.2.2 Hartree Products

Ex 2.2

$$\begin{aligned}
\mathscr{H}\Psi^{HP} &= \sum_{i=1}^{N} h(i)\chi_i(\mathbf{x}_1)\chi_j(\mathbf{x}_2)\cdots\chi_k(\mathbf{x}_N) \\
&= \varepsilon_i\chi_i(\mathbf{x}_1)\chi_j(\mathbf{x}_2)\cdots\chi_k(\mathbf{x}_N) + \chi_i(\mathbf{x}_1)[\varepsilon_j\chi_j(\mathbf{x}_2)]\cdots\chi_k(\mathbf{x}_N) + \cdots + \chi_i(\mathbf{x}_1)\chi_j(\mathbf{x}_2)\cdots[\varepsilon_k\chi_k(\mathbf{x}_N)] \\
&= (\varepsilon_i + \varepsilon_j + \cdots + \varepsilon_k)\Psi^{HP}
\end{aligned} \tag{2.2.9}$$

2.2.3 Slater Determinants

Ex 2.3

$$\begin{aligned}
\langle \Psi \,|\, \Psi \rangle &= \frac{1}{2}(\langle \chi_i \,|\, \chi_i \rangle \langle \chi_j \,|\, \chi_j \rangle - \langle \chi_i \,|\, \chi_j \rangle \langle \chi_j \,|\, \chi_i \rangle - \langle \chi_j \,|\, \chi_i \rangle \langle \chi_i \,|\, \chi_j \rangle + \langle \chi_j \,|\, \chi_j \rangle \langle \chi_i \,|\, \chi_i \rangle) \\
&= \frac{1}{2}(1 + 0 + 0 + 1) = 1
\end{aligned} \tag{2.2.10}$$

Ex 2.4 According to Ex. 2.2, we know that $\chi_i(\mathbf{x}_1)\chi_j(\mathbf{x}_2)$ are an eigenfunction of $\mathscr{H}$ and has the eigenvalue $\varepsilon_i\varepsilon_j$. Similarly, we have the same conclusion for $\chi_i(\mathbf{x}_2)\chi_j(\mathbf{x}_1)$.
For the antisymmetrized wave function,

$$\begin{aligned}
\langle \Psi \,|\, \mathscr{H} \,|\, \Psi \rangle = \frac{1}{2}\,(&\langle \chi_i(\mathbf{x}_1)\chi_j(\mathbf{x}_2) \,|\, \mathscr{H} \,|\, \chi_i(\mathbf{x}_1)\chi_j(\mathbf{x}_2) \rangle - \langle \chi_i(\mathbf{x}_1)\chi_j(\mathbf{x}_2) \,|\, \mathscr{H} \,|\, \chi_j(\mathbf{x}_1)\chi_i(\mathbf{x}_2) \rangle \\
&- \langle \chi_j(\mathbf{x}_1)\chi_i(\mathbf{x}_2) \,|\, \mathscr{H} \,|\, \chi_i(\mathbf{x}_1)\chi_j(\mathbf{x}_2) \rangle + \langle \chi_j(\mathbf{x}_1)\chi_i(\mathbf{x}_2) \,|\, \mathscr{H} \,|\, \chi_j(\mathbf{x}_1)\chi_i(\mathbf{x}_2) \rangle) \\
= \frac{1}{2}&(\varepsilon_i + \varepsilon_j - 0 - 0 + \varepsilon_i + \varepsilon_j) \\
= \varepsilon_i& + \varepsilon_j
\end{aligned} \tag{2.2.11}$$

Ex 2.5

$$\begin{aligned}\langle K \mid L\rangle &= \frac{1}{2}\left\langle \chi_i(\mathbf{x}_1)\chi_j(\mathbf{x}_2) - \chi_j(\mathbf{x}_1)\chi_i(\mathbf{x}_2) \,\middle|\, \chi_k(\mathbf{x}_1)\chi_l(\mathbf{x}_2) - \chi_l(\mathbf{x}_1)\chi_k(\mathbf{x}_2)\right\rangle \\ &= \frac{1}{2}(\langle\chi_i \mid \chi_k\rangle\langle\chi_j \mid \chi_l\rangle - \langle\chi_i \mid \chi_l\rangle\langle\chi_j \mid \chi_k\rangle - \langle\chi_j \mid \chi_k\rangle\langle\chi_i \mid \chi_l\rangle + \langle\chi_j \mid \chi_l\rangle\langle\chi_i \mid \chi_k\rangle) \\ &= \frac{1}{2}(\delta_{ik}\delta_{jl} - \delta_{il}\delta_{jk} - \delta_{jk}\delta_{il} + \delta_{jl}\delta_{ik}) \\ &= \delta_{ik}\delta_{jl} - \delta_{il}\delta_{jk}\end{aligned} \tag{2.2.12}$$

2.2.4 The Hartree-Fock Approximation

2.2.5 The Minimal Basis H_2 Model

Ex 2.6

$$\langle\psi_1 \mid \psi_1\rangle = \frac{1}{2(1+S_{12})}(\langle\phi_1 \mid \phi_1\rangle + 2\langle\phi_1 \mid \phi_2\rangle + \langle\phi_2 \mid \phi_2\rangle) = \frac{2+2S_{12}}{2(1+S_{12})} = 1 \tag{2.2.13}$$

$$\langle\psi_2 \mid \psi_2\rangle = \frac{1}{2(1-S_{12})}(\langle\phi_1 \mid \phi_1\rangle - 2\langle\phi_1 \mid \phi_2\rangle + \langle\phi_2 \mid \phi_2\rangle) = \frac{2-2S_{12}}{2(1-S_{12})} = 1 \tag{2.2.14}$$

$$\langle\psi_1 \mid \psi_2\rangle = \frac{1}{2\sqrt{1+S_{12}}\sqrt{1-S_{12}}}(\langle\phi_1 \mid \phi_1\rangle - \langle\phi_2 \mid \phi_2\rangle) = 0 \tag{2.2.15}$$

2.2.6 Excited Determinants

2.2.7 Form of the Exact Wfn and CI

Ex 2.7 Size of full CI matrix

$$C_{72}^{42} = 164307576757973059488 \approx 1.64 \times 10^{20} \tag{2.2.16}$$

The number of singly excited determinants

$$42 \times 30 = 1260 \tag{2.2.17}$$

The number of doubly excited determinants

$$C_{42}^{2}C_{30}^{2} = 374535 \tag{2.2.18}$$

2.3 Operators and Matrix Elements

2.3.1 Minimal Basis H_2 Matrix Elements

Ex 2.8

$$\begin{aligned}\left\langle\Psi_{12}^{34} \,\middle|\, h(1) \,\middle|\, \Psi_{12}^{34}\right\rangle &= \frac{1}{2}\left\langle\chi_3(\mathbf{x}_1)\chi_4(\mathbf{x}_2) - \chi_3(\mathbf{x}_2)\chi_4(\mathbf{x}_1) \,\middle|\, h(1) \,\middle|\, \chi_3(\mathbf{x}_1)\chi_4(\mathbf{x}_2) - \chi_3(\mathbf{x}_2)\chi_4(\mathbf{x}_1)\right\rangle \\ &= \frac{1}{2}(\langle\chi_3 \mid h(1) \mid \chi_3\rangle - 0 - 0 + \langle\chi_4 \mid h(1) \mid \chi_4\rangle) \\ &= \frac{1}{2}(\langle\chi_3 \mid h(1) \mid \chi_3\rangle + \langle\chi_4 \mid h(1) \mid \chi_4\rangle)\end{aligned} \tag{2.3.1}$$

thus

$$\left\langle\Psi_{12}^{34} \,\middle|\, \mathcal{O}_1 \,\middle|\, \Psi_{12}^{34}\right\rangle = \langle 3 \mid h \mid 3\rangle + \langle 4 \mid h \mid 4\rangle \tag{2.3.2}$$

$$\begin{aligned}\left\langle\Psi_0 \,\middle|\, h(1) \,\middle|\, \Psi_{12}^{34}\right\rangle &= \frac{1}{2}\left\langle\chi_1(\mathbf{x}_1)\chi_2(\mathbf{x}_2) - \chi_2(\mathbf{x}_2)\chi_1(\mathbf{x}_1) \,\middle|\, h(1) \,\middle|\, \chi_3(\mathbf{x}_1)\chi_4(\mathbf{x}_2) - \chi_3(\mathbf{x}_2)\chi_4(\mathbf{x}_1)\right\rangle \\ &= \frac{1}{2}(0 - 0 - 0 + 0) \\ &= 0\end{aligned} \tag{2.3.3}$$

thus

$$\left\langle\Psi_0 \,\middle|\, \mathcal{O}_1 \,\middle|\, \Psi_{12}^{34}\right\rangle = 0 \tag{2.3.4}$$

Similarly, we get

$$\left\langle\Psi_{12}^{34} \,\middle|\, \mathcal{O}_1 \,\middle|\, \Psi_0\right\rangle = 0 \tag{2.3.5}$$

Ex 2.9 From Eq. (2.92) in textbook, we get

$$\langle \Psi_0 \,|\, \mathscr{H} \,|\, \Psi_0 \rangle = \langle 1 \,|\, h \,|\, 1 \rangle + \langle 2 \,|\, h \,|\, 2 \rangle + \langle 12 \,|\, 12 \rangle - \langle 12 \,|\, 21 \rangle \tag{2.3.6}$$

From Ex 2.8, we get

$$\left\langle \Psi_0 \,\middle|\, \mathcal{O}_1 \,\middle|\, \Psi_{12}^{34} \right\rangle = \left\langle \Psi_{12}^{34} \,\middle|\, \mathcal{O}_1 \,\middle|\, \Psi_0 \right\rangle = 0 \tag{2.3.7}$$

thus

$$\begin{aligned}
\left\langle \Psi_0 \,\middle|\, \mathscr{H} \,\middle|\, \Psi_{12}^{34} \right\rangle &= \left\langle \Psi_0 \,\middle|\, \mathcal{O}_2 \,\middle|\, \Psi_{12}^{34} \right\rangle \\
&= \frac{1}{2} \left\langle \chi_1(\mathbf{x}_1)\chi_2(\mathbf{x}_2) - \chi_1(\mathbf{x}_2)\chi_2(\mathbf{x}_1) \,\middle|\, \frac{1}{r_{12}} \,\middle|\, \chi_3(\mathbf{x}_1)\chi_4(\mathbf{x}_2) - \chi_3(\mathbf{x}_2)\chi_4(\mathbf{x}_1) \right\rangle \\
&= \langle 12 \,|\, 34 \rangle - \langle 12 \,|\, 43 \rangle
\end{aligned} \tag{2.3.8}$$

$$\begin{aligned}
\left\langle \Psi_{12}^{34} \,\middle|\, \mathscr{H} \,\middle|\, \Psi_0 \right\rangle &= \left\langle \Psi_{12}^{34} \,\middle|\, \mathcal{O}_2 \,\middle|\, \Psi_0 \right\rangle \\
&= \frac{1}{2} \left\langle \chi_3(\mathbf{x}_1)\chi_4(\mathbf{x}_2) - \chi_3(\mathbf{x}_2)\chi_4(\mathbf{x}_1) \,\middle|\, \frac{1}{r_{12}} \,\middle|\, \chi_1(\mathbf{x}_1)\chi_2(\mathbf{x}_2) - \chi_2(\mathbf{x}_2)\chi_1(\mathbf{x}_1) \right\rangle \\
&= \langle 34 \,|\, 12 \rangle - \langle 34 \,|\, 21 \rangle
\end{aligned} \tag{2.3.9}$$

$$\begin{aligned}
\left\langle \Psi_{12}^{34} \,\middle|\, \mathscr{H} \,\middle|\, \Psi_{12}^{34} \right\rangle &= \left\langle \Psi_{12}^{34} \,\middle|\, h(1) + h(2) + \frac{1}{r_{12}} \,\middle|\, \Psi_{12}^{34} \right\rangle \\
&= 2 \times \frac{1}{2} \left\langle \chi_3(\mathbf{x}_1)\chi_4(\mathbf{x}_2) - \chi_3(\mathbf{x}_2)\chi_4(\mathbf{x}_1) \,\middle|\, h(1) \,\middle|\, \chi_3(\mathbf{x}_1)\chi_4(\mathbf{x}_2) - \chi_3(\mathbf{x}_2)\chi_4(\mathbf{x}_1) \right\rangle \\
&+ \frac{1}{2} \left\langle \chi_3(\mathbf{x}_1)\chi_4(\mathbf{x}_2) - \chi_3(\mathbf{x}_2)\chi_4(\mathbf{x}_1) \,\middle|\, \frac{1}{r_{12}} \,\middle|\, \chi_3(\mathbf{x}_1)\chi_4(\mathbf{x}_2) - \chi_3(\mathbf{x}_2)\chi_4(\mathbf{x}_1) \right\rangle \\
&= \langle 3 \,|\, h \,|\, 3 \rangle + \langle 4 \,|\, h \,|\, 4 \rangle + \langle 34 \,|\, 34 \rangle - \langle 34 \,|\, 43 \rangle
\end{aligned} \tag{2.3.10}$$

2.3.2 Notations for 1- and 2-Electron Integrals

2.3.3 General Rules for Matrix Elements

Ex 2.10

$$\langle K \,|\, \mathscr{H} \,|\, K \rangle = \sum_m^N [m|h|m] + \frac{1}{2} \sum_m^N \sum_n^N \langle mn \,\|\, mn \rangle = \sum_m^N [m|h|m] + \frac{1}{2} \sum_m^N \sum_n^N ([mm|nn] - [mn|nm]) \tag{2.3.11}$$

When $m = n$,

$$[mm|mm] - [mm|mm] = 0 \tag{2.3.12}$$

thus

$$\langle K \,|\, \mathscr{H} \,|\, K \rangle = \sum_m^N [m|h|m] + \frac{1}{2} \sum_m^N \sum_{n \neq m}^N ([mm|nn] - [mn|nm]) = \sum_m^N [m|h|m] + \sum_m^N \sum_{n > m}^N ([mm|nn] - [mn|nm]) \tag{2.3.13}$$

Ex 2.11

$$\begin{aligned}
\langle K \,|\, \mathscr{H} \,|\, K \rangle = \langle K \,|\, \mathcal{O}_1 + \mathcal{O}_2 \,|\, K \rangle &= \sum_m^N [m|h|m] + \sum_m^N \sum_{n > m}^N \langle mn \,\|\, mn \rangle \\
&= \langle 1 \,|\, h \,|\, 1 \rangle + \langle 2 \,|\, h \,|\, 2 \rangle + \langle 3 \,|\, h \,|\, 3 \rangle + \langle 12 \,\|\, 12 \rangle + \langle 13 \,\|\, 13 \rangle + \langle 23 \,\|\, 23 \rangle
\end{aligned} \tag{2.3.14}$$

Ex 2.12

$$\begin{aligned}
\langle \Psi_0 \,|\, \mathscr{H} \,|\, \Psi_0 \rangle &= \langle 1 \,|\, h \,|\, 1 \rangle + \langle 2 \,|\, h \,|\, 2 \rangle + \langle 12 \,\|\, 12 \rangle \\
&= \langle 1 \,|\, h \,|\, 1 \rangle + \langle 2 \,|\, h \,|\, 2 \rangle + \langle 12 \,|\, 12 \rangle - \langle 12 \,|\, 21 \rangle
\end{aligned} \tag{2.3.15}$$

$$\left\langle \Psi_0 \,\middle|\, \mathscr{H} \,\middle|\, \Psi_{12}^{34} \right\rangle = \langle 12 \,\|\, 34 \rangle = \langle 12 \,|\, 34 \rangle - \langle 12 \,|\, 43 \rangle \tag{2.3.16}$$

$$\left\langle \Psi_{12}^{34} \,\middle|\, \mathscr{H} \,\middle|\, \Psi_0 \right\rangle = \langle 34 \,\|\, 12 \rangle = \langle 34 \,|\, 12 \rangle - \langle 34 \,|\, 21 \rangle \tag{2.3.17}$$

$$\begin{aligned}
\left\langle \Psi_{12}^{34} \,\middle|\, \mathscr{H} \,\middle|\, \Psi_{12}^{34} \right\rangle &= \langle 3 \,|\, h \,|\, 3 \rangle + \langle 4 \,|\, h \,|\, 4 \rangle + \langle 34 \,\|\, 34 \rangle \\
&= \langle 3 \,|\, h \,|\, 3 \rangle + \langle 4 \,|\, h \,|\, 4 \rangle + \langle 34 \,|\, 34 \rangle - \langle 34 \,|\, 43 \rangle
\end{aligned} \tag{2.3.18}$$

Which are exactly the same with Ex 2.9.

Ex 2.13 if $a = b$, $r = s$

$$\langle \Psi_a^r \,|\, \mathcal{O} \,|\, \Psi_b^s \rangle = \langle \Psi_a^r \,|\, \mathcal{O}_1 \,|\, \Psi_a^r \rangle = \sum_c^N \langle c \,|\, h \,|\, c \rangle - \langle a \,|\, h \,|\, a \rangle + \langle r \,|\, h \,|\, r \rangle \tag{2.3.19}$$

if $a = b$, $r \neq s$

$$\langle \Psi_a^r \,|\, \mathcal{O} \,|\, \Psi_b^s \rangle = \langle \Psi_a^r \,|\, \mathcal{O}_1 \,|\, \Psi_a^s \rangle = \langle r \,|\, h \,|\, s \rangle \tag{2.3.20}$$

if $a \neq b$, $r = s$

$$\langle \Psi_a^r \,|\, \mathcal{O} \,|\, \Psi_b^s \rangle = \langle \Psi_a^r \,|\, \mathcal{O}_1 \,|\, \Psi_b^r \rangle = \langle \Psi_a^r \,|\, \mathcal{O}_1 \,|\, -(\Psi_a^r)_b^a \rangle = -\langle b \,|\, h \,|\, a \rangle \tag{2.3.21}$$

if $a \neq b$, $r \neq s$

$$\langle \Psi_a^r \,|\, \mathcal{O} \,|\, \Psi_b^s \rangle = \langle \Psi_a^r \,|\, \mathcal{O}_1 \,|\, (\Psi_a^r)_{rb}^{as} \rangle = 0 \tag{2.3.22}$$

Ex 2.14

$${}^N E_0 = \sum_m^N \langle m \,|\, h \,|\, m \rangle + \sum_m^M \sum_{n>m}^M \langle mn \,\|\, mn \rangle \tag{2.3.23}$$

$${}^{N-1} E_0 = \sum_{m \neq a}^N \langle m \,|\, h \,|\, m \rangle + \sum_{m \neq a}^M \sum_{n>m, n \neq a}^M \langle mn \,\|\, mn \rangle \tag{2.3.24}$$

$${}^N E_0 - {}^{N-1} E_0 = \langle a \,|\, h \,|\, a \rangle + \sum_{b \neq a}^N \langle ab \,\|\, ab \rangle \tag{2.3.25}$$

2.3.4 Derivation of the Rules for Matrix Elements

Ex 2.15

$$\begin{aligned} \langle \Psi \,|\, \mathscr{H} \,|\, \Psi \rangle &= \frac{1}{N!} \left\langle \sum_{n=1}^{N!} (-1)^{p_n} \mathscr{P}_n \{\chi_i(1)\chi_j(2)\cdots\chi_k(N)\} \,\middle|\, \sum_{c=1}^N h(c) \,\middle|\, \sum_{m=1}^{N!} (-1)^{p_m} \mathscr{P}_m \{\chi_i(1)\chi_j(2)\cdots\chi_k(N)\} \right\rangle \\ &= \frac{1}{N!} \sum_{n=1}^{N!} \sum_{m=1}^{N!} (-1)^{p_n+p_m} \sum_{c=1}^N \langle \mathscr{P}_n \{\chi_i(1)\chi_j(2)\cdots\chi_k(N)\} \,|\, h(c) \,|\, \mathscr{P}_m \{\chi_i(1)\chi_j(2)\cdots\chi_k(N)\} \rangle \end{aligned} \tag{2.3.26}$$

Since the integral inside equals 0 when $\mathscr{P}_n \neq \mathscr{P}_m$,

$$\langle \Psi \,|\, \mathscr{H} \,|\, \Psi \rangle = \frac{1}{N!} \sum_{n=1}^{N!} (-1)^{p_n+p_n} (\varepsilon_i + \varepsilon_j + \cdots + \varepsilon_k) = \varepsilon_i + \varepsilon_j + \cdots + \varepsilon_k \tag{2.3.27}$$

Ex 2.16 Suppose

$$c = \langle K^{HP} \,|\, \mathscr{H} \,|\, L \rangle = \left\langle K^{HP} \,\middle|\, \mathscr{H} \,\middle|\, \sum_{m=1}^{N!} (-1)^{p_m} \mathscr{P}_m L^{HP} \right\rangle \tag{2.3.28}$$

thus

$$\langle K \,|\, \mathscr{H} \,|\, L \rangle = \sum_{n=1}^{N!} (-1)^{p_n} \left\langle \mathscr{P}_n K^{HP} \,\middle|\, \mathscr{H} \,\middle|\, \sum_{m=1}^{N!} (-1)^{p_m} \mathscr{P}_m L^{HP} \right\rangle \tag{2.3.29}$$

2.3.5 Transition from Spin Orbitals to Spatial Orbitals

Ex 2.17

$$\begin{aligned} |1\rangle &= |\psi_1 \alpha\rangle \quad |2\rangle = |\psi_1 \beta\rangle \\ |3\rangle &= |\psi_2 \alpha\rangle \quad |4\rangle = |\psi_2 \beta\rangle \end{aligned} \tag{2.3.30}$$

thus

$$\begin{aligned} \mathbf{H} &= \begin{pmatrix} \langle 1 \,|\, h \,|\, 1 \rangle + \langle 2 \,|\, h \,|\, 2 \rangle + \langle 12 \,|\, 12 \rangle - \langle 12 \,|\, 21 \rangle & \langle 12 \,|\, 34 \rangle - \langle 12 \,|\, 43 \rangle \\ \langle 34 \,|\, 12 \rangle - \langle 34 \,|\, 21 \rangle & \langle 3 \,|\, h \,|\, 3 \rangle + \langle 4 \,|\, h \,|\, 4 \rangle + \langle 34 \,|\, 34 \rangle - \langle 34 \,|\, 43 \rangle \end{pmatrix} \\ &= \begin{pmatrix} 2(1|h|1) + (11|11) & (12|12) \\ (21|21) & 2(2|h|2) + (22|22) \end{pmatrix} \end{aligned} \tag{2.3.31}$$

Ex 2.18