LECTURE 19

The Transition Matrix as a change of Coordinates

(a) Exemplified

(b) Defined

(c) Discussed

(d) Its effect on a Linear Transformation

The Concept of a Transition Matrix

(= Change of Coordinates)

Example 19.1 (Molecules and Atoms)

A) Consider a given amount of mass, a mixture of gaseous compounds consisting of methane (CH_4), oxygen (O_2), and water (H_2O). Such a mixture is expressed mathematically by by the vector

$$\vec{u} = x_1 \overrightarrow{CH_4} + x_2 \overrightarrow{O_2} + x_3 \overrightarrow{H_2O}$$

where x_1, x_2 and x_3 are the amounts of each compound expressed in terms moles (multiples of Avogado's number).

B) Subjecting this mixture to a dissociation reaction (typically requiring a fair

amount of energy), one find that the mixture of molecular compounds becomes a mixture of atomic carbon (C) hydrogen (H) and oxygen (O):

$$\vec{u} = x_1' \vec{C} + x_2' \vec{H} + x_3' \vec{O} \qquad (*)$$

C) Chemical analysis of each molecular compound reveals that

$$\left.\begin{aligned} \overrightarrow{CH_4} &= \vec{C} + 4\vec{H} \\ \overrightarrow{O_2} &= 2\vec{O} \\ \overrightarrow{H_2O} &= 2\vec{H} + \vec{O} \end{aligned}\right\} (**)$$

D) Thus the theory of the chemical atom ~~gives~~ demands the introduction of two alternative vectorial bases for characterizing the chemical nature of the given (vectorial) amount of mass:

"molecular" basis "atomic" basis

$B = \{\overrightarrow{CH_4}, \vec{O_2}, \overrightarrow{H_2O}\}$ and $C = \{\vec{C}, \vec{H}, \vec{O}\}$

Each basis serves as a multidimensional standard relative to which one expresses the composition of the given mass vector:

$$\overrightarrow{CH_4}x_1 + \vec{O_2}x_2 + \overrightarrow{H_2O}x_3 = \vec{U} = \vec{C}x_1' + \vec{H}x_2' + \vec{O}x_3'$$

E) The elements of the molecular and the atomic bases are related by Eq (**) on page 19.2. Consequently, one finds that

$$\vec{u} = (\vec{C} + 4\vec{H})x_1 + 2\vec{O}x_2 + (2\vec{H} + \vec{O})x_3$$

$$= \vec{C}x_1 + \vec{H}(4x_1 + 2x_3) + \vec{O}(2x_2 + x_3)$$

Comparing this with Eq.(*) on P 19.2 one finds that the atomic quantity of

the dissociated mixture is

$$\begin{aligned} x_1' &= x_1 \\ x_2' &= 4x_1 + 2x_3 \\ x_3' &= 2x_2 + x_3 \end{aligned} \quad \text{OR} \quad \begin{bmatrix} x_1' \\ x_2' \\ x_3' \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 4 & 0 & 2 \\ 0 & 2 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}$$

Here $\begin{bmatrix} x_1' \\ x_2' \\ x_3' \end{bmatrix} = [u]_B$ = "atomic representative of $\vec{u}$"

$\begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = [u]_C$ = "molecular repres've of $\vec{u}$"

$$\underbrace{\begin{bmatrix} 1 & 0 & 0 \\ 4 & 0 & 2 \\ 0 & 2 & 1 \end{bmatrix}}_{[P_{ij}]} = \left[[\overrightarrow{CH_4}]_C, [\vec{O_2}]_C, [\overrightarrow{H_2O}]_C \right] = P_{C \leftarrow B} = \text{"transition matrix from old B-basis to new C-basis"}$$

Thus $\boxed{x_i' = \sum_{j=1}^{3} P_{ij} x_j}$

~~The matrix $P_{C \leftarrow B}$ is the transition matrix from B to C; its column are the~~

Definition 19.1

Let $B = \{e_1, \dots, e_n\}$ be a basis for U

$C = \{e'_1, \dots, e'_n\}$ be another basis for U

The transition matrix $P_{C\leftarrow B}$ consists of the columns which are the C-representatives of the B-elements:

$$[P]_{C\leftarrow B} = \left[[\vec{e}_1]_C, \dots, [\vec{e}_n]_C \right]$$

For any vector $\vec{u} \in U$ one has

$$\boxed{[\vec{u}]_C = [P]_{C\leftarrow B}[\vec{u}]_B}$$ "matrix notation"

or

$$\boxed{x'_i = \sum_{j=1}^{n} P_{ij} x_j}$$ "index notation"

One has the following scheme

$$\begin{tikzcd}
 & U \arrow[dl, "u"', "\text{NEW basis } C"'] \arrow[dr, "\text{OLD basis } B"] & \\
\mathbb{R}^n & {[u]_C = [P]_{C\leftarrow B}[u]_B} & \mathbb{R}^n \arrow[ll, "{[P]_{C\leftarrow B}}"'] \\
\text{NEW} & & \text{OLD}
\end{tikzcd}$$

Figure 19.1 Transition matrix between old (B) and new (C) representations.

~~C-representatives of the B-basis vectors; one has~~

~~$\boxed{[\vec{u}]_C = [P]_{C \leftarrow B} [u]_B}$ or $\boxed{x'_i = \sum_{j=1}^{3} P_{ij}\, x_j}$~~

~~MATRIX NOTATION~~ ~~INDEX NOTATION~~

Parenthetical Comment:

On the other hand, the relation between the molecular and the atomic basis vectors, Eq.(**) on page 19.2 is

$$\overrightarrow{CH_4} = \vec{C} + 4\vec{H};\ \vec{O_2} = 2\vec{O};\ \overrightarrow{H_2O} = 2\vec{H} + \vec{O}$$

or

$$\underbrace{[\overrightarrow{CH_4}\ \vec{O_2}\ \overrightarrow{H_2O}]}_{\overset{\parallel\!|}{[B]}} = \underbrace{[\vec{C}\ \vec{H}\ \vec{O}]}_{\overset{\parallel\!|}{[C]}} \underbrace{\begin{bmatrix} 1 & 0 & 0 \\ 4 & 0 & 2 \\ 0 & 2 & 1 \end{bmatrix}}_{[P]_{C \leftarrow B}}$$

Thus, if one writes each basis as a row array, the same transition matrix

$[P]_{C \leftarrow B}$ can used to write

$$[B] = [C] P_{C \leftarrow B}. \qquad (\star)$$

and

$$\vec{u} = [B][u]_B = \overbrace{\underbrace{[C][P]_{C \leftarrow B}}_{[B]}[u]_B}^{[u]_C} \qquad (\star\star)$$

$$= [C][\vec{u}]_C \qquad (\star\star\star)$$

Note that in all of these equations the occurrence of a pair of repeated basis labels on one side of the equation, ~~guartees~~ guarantees that they do not appear on the other side. One can think of this as a kind of cancelation. This disappearance is a mathematical statement of the basis independence of the vector $\vec{u}$. More briefly one says that the vector $\vec{u}$ is a *geometrical* object.

PROBLEM:

What is the representation of this transformation relative to a new basis

$$C = \{\vec{e}'_1, \vec{e}'_2, \vec{e}'_3\}$$

related to the old basis B by mean of the transition matrix $[P]_{C\leftarrow B} \equiv P$

$$\begin{tikzcd}
& E^3 \arrow[dl, "C=\{e'_j\}"'] \arrow[dr, "B=\{e_i\}"] & \\
R^3 & & R^3 \arrow[ll, "{[P]_{C\leftarrow B} \equiv P}"']
\end{tikzcd}$$

$$[\vec{X}]_C = [P]_{C\leftarrow B}[X]_B \equiv P[X_B]$$

$$x'^j = \sum_{j=1}^{3} P_j{}^i x^i$$

Pictorially the problem is the following scheme:

$$\begin{tikzcd}
& & & U=E^3 \arrow[loop above, "T_{\vec{w}}"] \arrow[dlll, "C"'] \arrow[dl, "B"'] \arrow[dr, "B"] \arrow[drrr, "C"] & & & \\
R^3 \arrow[rr, shift right, "P^{-1}"'] \arrow[rrrrrr, bend right] & & R^3 \arrow[ll, shift right, "P"'] \arrow[rr, "{[Q]_B=[T_{\vec{w}}]_B}"'] & & R^3 \arrow[rr, "P"] & & R^3
\end{tikzcd}$$

$$[Q]_C \equiv [T_w]_C = ?$$

How is the representative $[T_w]_B$ related to the representative $[T]_C$ relative to the new basis $C = \{\vec{e}'_i\}$? The picture suggests

$$Q_C = P\, Q_B\, P^{-1}$$

The validity of this conjecture follows from the following constructive definitions

$$Q_C = \left[[T_{\vec{\omega}}(e'_1)]_C, \ldots, [T_{\vec{\omega}}(e'_3)]_C \right]$$

$$Q_B = \left[[T_{\vec{\omega}}(e_1)]_B, \ldots, [T_{\vec{\omega}}(\vec{e}_3)]_B \right]$$

and

$$P \equiv [P]_{C \leftarrow B} = \left[[e_1]_C, \ldots, [e_3]_C \right],$$

$$P^{-1} = \left[[e'_1]_B, \ldots, [e'_3]_B \right]$$

We have

$$Q_C = \left[[T_{\vec{\omega}}(\vec{e}'_1)]_C, \ldots, [T_{\vec{\omega}}(\vec{e}'_3)]_C \right]$$

$$= \left[P[T_{\vec{\omega}}(\vec{e}'_1)]_B, \ldots, P[T_{\vec{\omega}}(\vec{e}'_2)]_B \right] \quad \text{Def'n of P on P19,5}$$

$$= \left[P[T_\omega]_B[\vec{e}'_1]_B, \ldots, P[T_\omega]_B[\vec{e}'_3]_B \right] \quad \text{Rep'n Thm on P16,6}$$

$$= \left[P[T_\omega]_B P^{-1}[\vec{e}'_1]_C, \ldots, P[T_\omega]_B P^{-1}[e'_3] \right]$$

because $[u]_B = P^{-1}[u]_C$

$$= \left[P[T_\omega]_B P^{-1}\begin{bmatrix} 1 \\ \vdots \\ 0 \end{bmatrix}, \ldots, P[T_\omega]_B P^{-1}\begin{bmatrix} 0 \\ \vdots \\ 1 \end{bmatrix} \right]$$

Thus

$$Q_C = P\underbrace{[T_\omega]_B}_{Q_B} P^{-1}\begin{bmatrix} 1 & \cdots & 0 \\ & 1 & \vdots \\ 0 & \cdots & 1 \end{bmatrix}$$

$$\boxed{Q_C = P Q_B P^{-1}}$$

Comment:

The B representation of T_ω, Eq.(★) on P19.11, is

$$[\vec{v}]_B = [T_\omega]_B [\vec{X}]_B$$

Applying the coordinate transformation $P = [P]_{C \leftarrow B}$ and using its inverse P^{-1}, one obtains

$$P[\vec{v}]_B = P[T_\omega]P^{-1}P[X]_B$$

or

$$\boxed{[\vec{v}]_C = P T_\omega P^{-1} [X]_C}$$