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

Example 19.1

How does one mathematize Matter?

Let V = set of inventories of matter

= set of material entities/inventories

A) Consider a given amount of mass, a mixture consisting of

methane (CH_4)
oxygen (O_2)
water (H_2O)

Such a mixture is mathematized by the vector

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

(mixture in terms of molecules)

Here x_1, x_2, and x_3 are the amounts of each compound expressed in terms of 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):

$$\vec{U} = x_1' \vec{C} + x_2' \vec{H} + x_3' \vec{O} \quad \text{mixture in terms of atoms} \quad (*)$$

C) Chemical analysis of each molecular compound reveals that

$$\left.\begin{aligned} \overrightarrow{CH_4} &= \vec{C} + 4\vec{H} \\ \vec{O}_2 &= 2\vec{O} \\ \overrightarrow{H_2O} &= 2\vec{H} + \vec{O} \end{aligned}\right\} (**)$$

D) Thus the theory of the chemical atom 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 $\mathcal{C} = \{\vec{C}, \vec{H}, \vec{O}\}$

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

$$x'_1 = x_1$$
$$x'_2 = 4x_1 + 2x_3 \quad \text{OR} \quad \begin{bmatrix} x'_1 \\ x'_2 \\ x'_3 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 4 & 0 & 2 \\ 0 & 2 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}$$
$$x'_3 = 2x_2 + x_3$$

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 $\vec{u}$"

$$\underbrace{\begin{bmatrix} 1 & 0 & 0 \\ 4 & 0 & 2 \\ 0 & 2 & 1 \end{bmatrix}}_{[P_{ij}]} = \left[[\overrightarrow{CH_4}]_C, [\overrightarrow{O_2}]_C, [\overrightarrow{H_2O}]_C \right] =$$

$= P_{C \leftarrow B} =$ " 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 $B = \{e_1, \ldots, e_n\}$ be a basis for U

$C = \{e'_1, \ldots, e'_n\}$ 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:

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

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"

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

or

$$\underbrace{[\vec{CH_4} \;\; O_2 \;\; H_2O]}_{\substack{\parallel \\ [B]}} = \underbrace{[\vec{C} \;\; \vec{H} \;\; \vec{O}]}_{[C]} \underbrace{\begin{bmatrix} 1 & 0 & 0 \\ 4 & 0 & 2 \\ 0 & 2 & 1 \end{bmatrix}}_{P_{C\leftarrow B}}$$

i.e

$$\boxed{[B] = [C]\, P_{C\leftarrow B}}$$

Multiply both sides by the column vector

$$\begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}_B = [\vec{u}]_B$$

and obtain

$$\underbrace{[CH_4 \;\; O_2 \;\; H_2O]}_{[B]} \underbrace{\begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}}_{[u]_B} = \underbrace{[\vec{C} \;\; \vec{H} \;\; \vec{O}]}_{[C]} \underbrace{\underbrace{\begin{bmatrix} 1 & 0 & 0 \\ 4 & 0 & 2 \\ 0 & 2 & 1 \end{bmatrix}}_{P_{C\leftarrow B}} \underbrace{\begin{bmatrix} x^1 \\ x^2 \\ x^3 \end{bmatrix}}_{[u]_B}}_{\begin{bmatrix} x_1' \\ x_2' \\ x_3' \end{bmatrix}_C = [u]_C}$$

One obtains

$$[B][u]_B = [C]\, P_{C\leftarrow B} [u]_B$$

$$= [C][u]_C$$

Thus one has

$$[B][u]_B = \vec{u} = [C][u]_C$$

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

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

$$\overbrace{[P]_{C \leftarrow B}[u]_B}^{[u]_C}$$

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

Note that in all of these equations the occurrence of a pair of repeated basis labels on one side of the equation 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 <u>basis independence</u> of the vector $\vec{u}$. More briefly one says that the vector $\vec{u}$ is a geometrical object.

One has the following scheme

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

u

NEW basis C OLD basis B

$C = \{\vec{v}_1, \ldots, \vec{v}_n\}$ $B = \{\vec{u}_1, \ldots, \vec{u}_n\}$

$$[u]_C = [P]_{C\leftarrow B}[u]_B$$

NEW $[P]_{C\leftarrow B}$ OLD

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

$$\vec{v}_j d_j = \vec{u} = \vec{u}_i c_i \quad \Big| \quad \boxed{d_j = P_{ji} c_i}$$

$$= \vec{v}_j P_{ji} c_i \qquad [\vec{u}]_C = \begin{bmatrix} P_{1i} c_i \\ \vdots \\ P_{ni} c_i \end{bmatrix}$$

$$[C][\vec{u}]_C = \underbrace{[C][P]_{C\leftarrow B}}_{[B]}[\vec{u}]_B = [B][\vec{u}]_B$$

$$\boxed{\vec{v}_j = P_{ji}\vec{u}_i}$$