

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 given amount of mass)

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

$$\vec{u} = x_1 \vec{CH}_4 + x_2 \vec{O}_2 + x_3 \vec{H}_2\text{O}$$

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

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

amount of energy), one finds that the

mixture of molecular compounds becomes

a mixture of atomic carbon (C)

hydrogen (H) and oxygen (O):

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

c) Chemical analysis of each molecular compound reveals that

$$\left. \begin{aligned} \vec{CH}_4 &= \vec{C} + 4\vec{H} \\ \vec{O}_2 &= 2\vec{O} \\ \vec{H}_2\text{O} &= 2\vec{H} + \vec{O} \end{aligned} \right\} (**)$$

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

$$B = \{ \vec{C}, \vec{H}_4, \vec{O}_2, \vec{H}_2\vec{O} \} \text{ and } a = \{ \vec{C}, \vec{H}, \vec{O} \}$$

Each basis serves as a multidimensional standard relative to which one

expresses the composition of the given mass vector:

$$\vec{C}\vec{H}_4\vec{X}_1 + \vec{O}_2\vec{X}_2 + \vec{H}_2\vec{O}\vec{X}_3 = \vec{a} = \vec{C}\vec{X}_1 + \vec{H}\vec{X}_2 + \vec{O}\vec{X}_3$$

E) The elements of the molecular and the atomic bases are related by Eq. (*) on

page 19.2. Consequently, one finds that

$$\vec{a} = (\vec{C} + 4\vec{H})\vec{X}_1 + 2\vec{O}\vec{X}_2 + (2\vec{H} + \vec{O})\vec{X}_3 = \vec{C}\vec{X}_1 + \vec{H}(4\vec{X}_1 + 2\vec{X}_2) + \vec{O}(2\vec{X}_2 + \vec{X}_3)$$

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

the dissociated mixture is

$$\begin{aligned} X_1' &= X_1 \\ X_2' &= 4X_1 + 2X_3 \quad \text{OR} \\ X_3' &= 2X_2 + X_3 \end{aligned} \quad \text{OR} \quad \begin{bmatrix} X_1' \\ X_2' \\ X_3' \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 4 & 0 & 2 \\ 0 & 2 & 1 \end{bmatrix} \begin{bmatrix} X_1 \\ X_2 \\ X_3 \end{bmatrix}$$

Here

$$\begin{bmatrix} X_1' \\ X_2' \\ X_3' \end{bmatrix} = [u]_B = \text{"atomic representation of } \vec{a} \text{"}$$

$$\begin{bmatrix} X_1 \\ X_2 \\ X_3 \end{bmatrix} = [u]_C = \text{"molecular representation of } \vec{a} \text{"}$$

$$\begin{bmatrix} 1 & 0 & 0 \\ 4 & 0 & 2 \\ 0 & 2 & 1 \end{bmatrix} = \begin{bmatrix} [\vec{C}\vec{H}_4]_C \\ [\vec{O}_2]_C \\ [\vec{H}_2\vec{O}]_C \end{bmatrix} \begin{bmatrix} [\vec{C}]_B \\ [\vec{H}]_B \\ [\vec{O}]_B \end{bmatrix} =$$

Thus $[P_{ij}] = P_{C \leftarrow B} =$ "transition matrix from old B-basis to new C-basis"

$$X_i' = \sum_{j=1}^3 P_{ij} X_j$$

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

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Definition 19.1

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

$C = \{e'_1, \dots, e'_m\}$ be another basis for V

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

C -representatives of the B -elements:

$$[P]_{C \leftarrow B} = [[e'_1]_B, \dots, [e'_m]_B]$$

For any vector $u \in U$ one has

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

"matrix notation"

or

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

"index notation"

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One has the following scheme

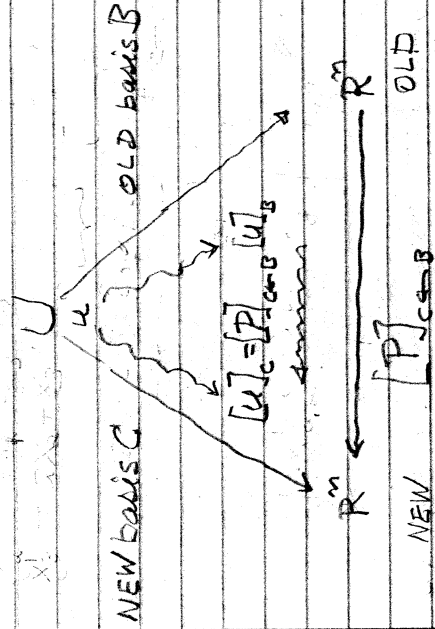


Figure 19.1 Transition matrix between

$old(B)$ and new(C) representing

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vector \vec{u} . More briefly one says that
the vector \vec{u} is a geometrical object.

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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 means of the

$$\text{transition matrix } [P]_{C \leftarrow B} \equiv P$$

$$C = \{\vec{e}_j\} \quad B = \{\vec{e}_i\}$$

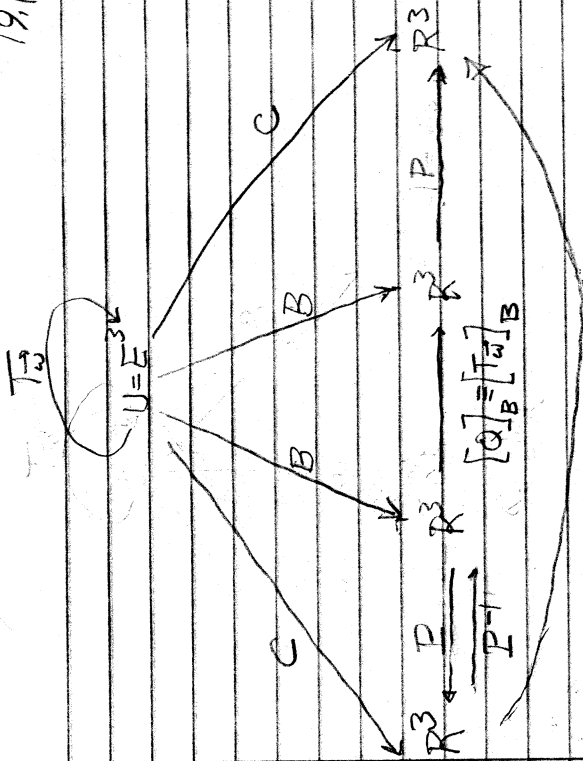
$$[x]_C = [P]_{C \leftarrow B} [x]_B \equiv P [x]_B$$

$$x^i = \sum_{j=1}^3 P^j_i x^j$$

Pictorially the problem is the following

scheme:

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

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

$$Q_C = P \circ_B P^{-1}$$

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The validity of this conjecture follows

from the following constructive definitions

$$Q_C = [T_{\vec{0}}(e_1)]_C, \dots, [T_{\vec{0}}(e_3)]_C$$

$$Q_B = [T_{\vec{0}}(e_1)]_B, \dots, [T_{\vec{0}}(e_3)]_B$$

and

$$P = [P]_{C \leftarrow B} = [e_1]_C, \dots, [e_3]_C$$

$$P^{-1} = [e_1]_B, \dots, [e_3]_B$$

We have

$$Q_C = [T_{\vec{0}}(e_1)]_C, \dots, [T_{\vec{0}}(e_3)]_C$$

$$= [P [T_{\vec{0}}(e_1)]_B, \dots, P [T_{\vec{0}}(e_3)]_B] \quad \text{Def'n of } P \text{ on P19.5}$$

$$= [P [T_{\vec{0}}(e_1)]_B, \dots, P [T_{\vec{0}}(e_3)]_B] \quad \text{Rephrasing on P16.6}$$

$$= [P [T_{\vec{0}}]_B P^{-1} [e_1]_C, \dots, P [T_{\vec{0}}]_B P^{-1} [e_3]_C]$$

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

$$= [P [T_{\vec{0}}]_B P^{-1} [0], \dots, P [T_{\vec{0}}]_B P^{-1} [1]]$$

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Thus

$$Q_C = P [T_{\vec{0}}]_B P^{-1} \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

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

Comment:

The B representation of $T_{\vec{0}}$, Eq. (8) on P19.11,

is

$$[T_{\vec{0}}]_B = [T_{\vec{0}}]_B [X]_B$$

Applying the coordinate transformation

$P = [P]_{C \leftarrow B}$ and using its

inverse P^{-1} , one obtains

$$P [T_{\vec{0}}]_B = P [T_{\vec{0}}]_B P^{-1} P [X]_B$$

or

$$[T_{\vec{0}}]_C = P [T_{\vec{0}}]_B P^{-1} [X]_C$$