Theoretische Chemie I

Prof. Martin Schütz

Wichtige Grundlagen der linearen Algebra

Uni Regensburg

Übungen (Teil 3)

WS 2013/14

Mathematik ist das Alphabet, mit dessen Hilfe Gott das Universum beschrieben hat
Galileo Galilei

Aufgabe 1

Verify the following relations for matrix exponentials:

a)

$$\exp(\mathbf{A})^\dagger = \exp(\mathbf{A}^\dagger)$$

b)

$$\mathbf{B}\exp(\mathbf{A})\mathbf{B}^{-1} = \exp(\mathbf{B}\mathbf{A}\mathbf{B}^{-1})$$

c)

$$\frac{\mathrm{d}}{\mathrm{d}\lambda}\exp(\lambda\mathbf{A}) = \mathbf{A}\exp(\lambda\mathbf{A}) = \exp(\lambda\mathbf{A})\mathbf{A}$$

provided the exponential of a matrix $\mathbf{A}$ is defined as

$$\exp(\mathbf{A}) = \sum_{n=0}^{\infty}\frac{\mathbf{A}^n}{n!}$$

Aufgabe 2

Let $\mathbf{D}$ be a diagonal matrix with diagonal elements d_i:

$$\mathbf{D} = \mathrm{diag}(d_1, d_2, ..., d_n) \tag{1}$$

$$\begin{pmatrix} d_1 & 0 & \cdots & 0 \\ 0 & d_2 & \cdots & 0 \\ \vdots & & \ddots & \vdots \\ 0 & 0 & \cdots & d_n \end{pmatrix} \tag{2}$$

(a) Show that the exponential of the diagonal matrix is given by:

$$\exp(\mathbf{D}) = \mathrm{diag}(\exp(d_1), \exp(d_2), ..., \exp(d_n)) \tag{3}$$

(b) Let $\mathbf{A}$ be a matrix that can be diagonalized:

$$\mathbf{A} = \mathbf{X}\mathbf{D}\mathbf{X}^{-1} \tag{4}$$

Verify the following relation for the determinant of the exponential of $\mathbf{A}$:

$$\det[\exp(\mathbf{A})] = \exp(\mathrm{Tr}\,\mathbf{A}) \tag{5}$$

where $\mathrm{Tr}\,\mathbf{A}$ is the trace of the matrix $\mathbf{A}$:

$$\mathrm{Tr}\,\mathbf{A} = \sum_{i=1}^{n} A_{ii} \tag{6}$$