Theoretische Chemie I
Wichtige Grundlagen der linearen Algebra
Lösungen (Teil 3)

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

Aufgabe 1

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

b) $Bexp(A)B^{-1} = B(\sum_{n=0}^{\infty} \frac{(A^n)}{n!})B^{-1} = \sum_{n=0}^{\infty} \frac{(BA^nB^{-1})}{n!} =$
$= \sum_{n=0}^{\infty} \frac{(BAB^{-1})^n}{n!} = exp(BAB^{-1})$
$[BB^{-1} = 1]$
$[BA^nB^{-1} = BAAA\cdots B^{-1} = BA1A1AB^{-1} =$
$= BAB^{-1}BAB^{-1}BA\cdots \ B^{-1} = (BAB^{-1})^n]$

c) $\frac{d}{d\lambda}exp(\lambda\ A) = \frac{d}{d\lambda}\sum_{n=0}^{\infty} \frac{(\lambda\ A)^n}{n!} = \frac{d}{d\lambda}\sum_{n=0}^{\infty} \frac{\lambda^n\ A^n}{n!} = \frac{d}{d\lambda}(1 + \sum_{n=1}^{\infty} \frac{\lambda^n\ A^n}{n!})$
$= \sum_{n=1}^{\infty} \frac{n\lambda^{n-1}\ A^n}{n!} = \sum_{n=1}^{\infty} \frac{\lambda^{n-1}\ A^n}{n-1!} = A(\sum_{n=1}^{\infty} \frac{\lambda^{n-1}\ A^{n-1}}{n-1!}) \overset{n'=n-1}{=} \sum_{n'=0}^{\infty} \frac{(\lambda\ A)^{n'}}{n'!} \overset{n'=n}{=}$
$= Aexp(\lambda\ A) = exp(\lambda\ A)A$

Aufgabe 2

a) $exp(D) = \sum_{n=0}^{\infty} \frac{D^n}{n!} = 1 + D + \frac{1}{2}D^2 + \frac{1}{3!}D^3 + ... =$
$= 1 + diag(d_1; d_2; ..) + \frac{1}{2}diag(d_1^2; d_2^2; ...) + ... =$
$= diag(1 + d_1 + \frac{1}{2}d_1^2 + ...\ ;\ 1 + d_2 + \frac{1}{2}d_2^2 + ...\ ;\ ...) =$
$= diag(\sum_{n=0}^{\infty} \frac{d_1^n}{n!}\ ;\ \sum_{n=0}^{\infty} \frac{d_2^n}{n!}\ ;\ ...) =$
$= diag(exp(d_1); diag(d_2); ...)$

b) $[det(AB) = detA \cdot detB]$
$[Tr(ABC) = Tr(CAB) = Tr(BCA)]$
$det(exp(A)) = det(exp(XDX^{-1})) \overset{A1}{=} det(Xexp(D)X^{-1}) =$
$= detX\ det(exp(D))\ det(X^{-1}) = det(XX^{-1})det(exp(D)) =$
$\overset{A2a)}{=} det(diag(exp(d_1); exp(d_2); ...)) =$
$= \prod_i exp(D_{ii}) = exp(\sum_i D_{ii}) = exp(Tr(D)) = exp(Tr(X^{-1}AX)) =$
$= exp(Tr(XX^{-1}A)) = exp(Tr(A))$