Functions of Matrices, transpose, Hermitian conjugate, trace

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From your power series lesson:

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

$$\sin(x) = \sum_{n=0}^{\infty} \frac{(-1)^n x^{2n+1}}{(2n+1)!}$$

$$\cos(x) = \sum_{n=0}^{\infty} \frac{(-1)^n x^{2n}}{(2n)!}$$

replace $x \to \hat{A}$, we have

$$\exp(\hat{A}) = \sum_{n=0}^{\infty} \frac{1}{n!}\hat{A}^n$$

$$\sin(\hat{A}) = \sum_{n=0}^{\infty} \frac{(-1)^n}{(2n+1)!}(\hat{A})^{2n+1}$$

$$\cos(\hat{A}) = \sum_{n=0}^{\infty} \frac{(-1)^n}{(2n)!}(\hat{A})^{2n}$$

Example: Consider one of the Pauli matrices, say

$$\hat{\sigma}_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

Express $\exp(i\theta_x\hat{\sigma}_x)$ as single 2x2 matrix

Note that θ_x is a real number

Solution:

$$\exp(i\theta_x\hat{\sigma}_x) = \sum_{n=0}^{\infty}\frac{(i\theta_x\hat{\sigma}_x)^n}{n!}$$

which we can rewrite by grouping the odd and even powers:

$$= \sum_{k=0}^{\infty}\left[\frac{(i\theta_x\hat{\sigma}_x)^{2k}}{(2k)!} + \frac{(i\theta_x\hat{\sigma}_x)^{2k+1}}{(2k+1)!}\right]$$

Notice that:

$$(i\theta_x\hat{\sigma}_x)^2 = i^2\theta_x^2\hat{\sigma}_x^2$$

$$= (-1)\theta_x^2\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

$$= -\theta_x^2\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$ ← an identity matrix in 2D

$$= -\theta_x^2 \mathbb{1}_{2\times2}$$

Thus, $$(i\theta_x\hat{\sigma}_x)^{2k} = \left[(i\theta_x\hat{\sigma}_x)^2\right]^k$$

$$= \left[-\theta_x^2\mathbb{1}_{2\times2}\right]^k$$

$$= \left[(-1)^k\theta_x^{2k}(\mathbb{1}_{2\times2})^k\right] \quad ; \quad \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}^k = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad \mathbb{1}_{2\times2}^k = \mathbb{1}_{2\times2}$$

$$= (-1)^k\theta_x^{2k}\mathbb{1}_{2\times2}$$

Also, $$(i\theta_x\hat{\sigma}_x)^{2k+1} = (i\theta_x\hat{\sigma}_x)^{2k}(i\theta_x\hat{\sigma}_x)$$

$$= (-1)^k\theta_x^{2k}\mathbb{1}_{2\times2}\cdot(i\theta_x\hat{\sigma}_x)$$

$$= i(-1)^k\theta_x^{2k+1}\hat{\sigma}_x \qquad \mathbb{1}_{2\times2}\hat{\sigma}_x = \hat{\sigma}_x$$

Accomplishment so far: all matrices are no longer raised to some power.

$$\exp(i\theta_x\hat{\sigma}_x) = \sum_{k=0}^{\infty}\left[\frac{(i\theta_x\hat{\sigma}_x)^{2k}}{(2k)!} + \frac{(i\theta_x\hat{\sigma}_x)^{2k+1}}{(2k+1)!}\right]$$

$$= \sum_{k=0}^{\infty}\left[\frac{(-1)^k\theta_x^{2k}}{(2k)!}\mathbb{1}_{2\times2} + i\frac{(-1)^k\theta_x^{2k+1}}{(2k+1)!}\hat{\sigma}_x\right]$$

$$= \left[\sum_{k=0}^{\infty}\frac{(-1)^k\theta_x^{2k}}{(2k)!}\right]\mathbb{1}_{2\times2} + i\left[\sum_{k=0}^{\infty}\frac{(-1)^k\theta_x^{2k+1}}{(2k+1)!}\right]\hat{\sigma}_x$$

$$= (\cos\theta_x)\mathbb{1}_{2\times2} + i(\sin\theta_x)\hat{\sigma}_x$$

$$= (\cos\theta_x)\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + i(\sin\theta_x)\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

$$\exp(i\theta_x\hat{\sigma}_x) = \begin{pmatrix} \cos\theta_x & i\sin\theta_x \\ i\sin\theta_x & \cos\theta_x \end{pmatrix}$$

Q1. Do the above evaluation with $\exp(i\theta_y\hat{\sigma}_y)$ and $\exp(i\theta_z\hat{\sigma}_z)$ where θ_y and θ_z are real numbers.

The Baker-Campbell-Hausdorff (BCH) formula

* $$\exp(\hat{X})\exp(\hat{Y}) = \exp(\hat{Z})$$

where $$\hat{Z} = \hat{X} + \hat{Y} + \frac{1}{2}[\hat{X},\hat{Y}] + \frac{1}{12}\left([\hat{X},[\hat{X},\hat{Y}]] + [\hat{Y},[\hat{Y},\hat{X}]]\right) + \dots$$

when $[\hat{X},\hat{Y}] = 0$, then

$$\exp(\hat{X})\exp(\hat{Y}) = \exp(\hat{X}+\hat{Y})$$

* $$\exp(-\hat{T})\hat{A}\exp(\hat{T}) = \hat{A} + [\hat{A},\hat{T}] + \frac{1}{2!}[[\hat{A},\hat{T}],\hat{T}] + \frac{1}{3!}[[[\hat{A},\hat{T}],\hat{T}],\hat{T}] + \dots$$

Example:

say $\hat{T} = -i\frac{\theta}{2}\hat{\sigma}_z$

$$\exp\left(i\tfrac{\theta}{2}\hat{\sigma}_z\right)\hat{\sigma}_x\exp\left(-i\tfrac{\theta}{2}\hat{\sigma}_z\right) = \hat{\sigma}_x + \left(-i\tfrac{\theta}{2}\right)[\hat{\sigma}_x,\hat{\sigma}_z] + \left(-i\tfrac{\theta}{2}\right)^2\frac{1}{2!}[[\hat{\sigma}_x,\hat{\sigma}_z],\hat{\sigma}_z] + \left(-i\tfrac{\theta}{2}\right)^3\frac{1}{3!}[[[\hat{\sigma}_x,\hat{\sigma}_z],\hat{\sigma}_z],\hat{\sigma}_z] + \dots$$

Note that: $[\hat{\sigma}_x, \hat{\sigma}_z] = -2i\hat{\sigma}_y$

$[\hat{\sigma}_y, \hat{\sigma}_z] = +2i\sigma_x$

$$= \hat{\sigma}_x + \left(-i\tfrac{\theta}{2}\right)(-2i\hat{\sigma}_y) + \left(-i\tfrac{\theta}{2}\right)^2\frac{1}{2!}[-2i\hat{\sigma}_y,\hat{\sigma}_z] + \left(-i\tfrac{\theta}{2}\right)^3\frac{1}{3!}[[-2i\hat{\sigma}_y,\hat{\sigma}_z],\hat{\sigma}_z] + \dots$$

$$= \hat{\sigma}_x + \left(-i\tfrac{\theta}{2}\right)(-2i\hat{\sigma}_y) + \left(-i\tfrac{\theta}{2}\right)^2\frac{1}{2!}(-2i)[\hat{\sigma}_y,\hat{\sigma}_z] + \left(-i\tfrac{\theta}{2}\right)^3\frac{1}{3!}(-2i)[[\hat{\sigma}_y,\hat{\sigma}_z],\hat{\sigma}_z] + \dots$$

$$= \hat{\sigma}_x + \left(-i\tfrac{\theta}{2}\right)(-2i\hat{\sigma}_y) + \left(-i\tfrac{\theta}{2}\right)^2\frac{1}{2!}(-2i)(+2i)\hat{\sigma}_x + \left(-i\tfrac{\theta}{2}\right)^3\frac{1}{3!}(-2i)[\cancel{+2i\hat{\sigma}_x,\hat{\sigma}_z}] \to (+2i)(-2i\hat{\sigma}_y) + \dots$$

EVEN TERMS: $$\left(-i\tfrac{\theta}{2}\right)^{2k}\frac{1}{(2k)!}(2)^{2k}\hat{\sigma}_x$$

$$= \frac{(-1)^k\theta^{2k}}{(2k)!}\hat{\sigma}_x$$

ODD TERMS: $$\left(-i\tfrac{\theta}{2}\right)^{2k+1}\frac{(-i)(2)^{2k+1}}{(2k+1)!}\hat{\sigma}_y$$

$$= \frac{(-i)(-1)^k(-i)\theta^{2k+1}}{(2k+1)!}\hat{\sigma}_y$$

$$= -\frac{(-1)^k\theta^{2k+1}}{(2k+1)!}\hat{\sigma}_y$$

$$\exp\left(i\tfrac{\theta}{2}\hat{\sigma}_z\right)\hat{\sigma}_x\exp\left(-i\tfrac{\theta}{2}\hat{\sigma}_z\right) = \sum_{k=0}^{\infty}\frac{(-1)^k\theta^{2k}}{(2k)!}\hat{\sigma}_x - \sum_{k=0}^{\infty}\frac{(-1)^k\theta^{2k+1}}{(2k+1)!}\hat{\sigma}_y$$

We recognize the series:

$$= \cos\theta\cdot\hat{\sigma}_x - \sin\theta\cdot\hat{\sigma}_y$$

Q2. Reduce

$$\exp\left(i\tfrac{\theta}{2}\hat{\sigma}_z\right)\hat{\sigma}_y\exp\left(-i\tfrac{\theta}{2}\hat{\sigma}_z\right)$$

in terms of a superposed Pauli matrices with no commutators.
Do this using two methods:
a) using BCH formula
b) using the result of Q1.

Transpose of a Matrix

Given a matrix $\hat{A}$, (with elements A_{ij}) the transpose of $\hat{A}$ (denoted by $\hat{A}^T$) will have entries given by

$$(\hat{A}^T)_{ij} = \hat{A}_{ji}$$

If $\hat{A}$ is an $M\times N$ matrix, then $\hat{A}^T$ is an $N\times M$.

let $\hat{C}_{ij} = A_{ij} + B_{ij}$

$$\hat{C}^T \to (\hat{C}^T)_{ij} = C_{ji}$$

$$= A_{ji} + B_{ji}$$

but $A_{ji} = (\hat{A}^T)_{ij}$ and $B_{ji} = (\hat{B}^T)_{ij}$

$$(\hat{C}^T)_{ij} = (\hat{A}^T)_{ij} + (\hat{B}^T)_{ij}$$

or $$[(\hat{A}+\hat{B})^T]_{ij} = (\hat{A}^T)_{ij} + (\hat{B}^T)_{ij}$$

Transpose of a product

$$(\hat{A}\hat{B})^T = [(\hat{A}\hat{B})^T]_{ij}$$

$$= (\hat{A}\hat{B})_{ji}$$

$$= \sum_{k=1}^{N} A_{jk}B_{ki}$$

$$= \sum_{k=1}^{N}(\hat{A}^T)_{kj}(\hat{B}^T)_{ik}$$ ← this is not the proper ordering to define a product

$$= \sum_{k=1}^{N}(\hat{B}^T)_{ik}(\hat{A}^T)_{kj}$$

$$= (\hat{B}^T\hat{A}^T)_{ij}$$

$$(\hat{A}\hat{B})^T = \hat{B}^T\hat{A}^T$$

It follows that:

$$(\hat{A}\hat{B}\hat{C}\dots\hat{Z})^T = \hat{Z}^T\dots\hat{C}^T\hat{B}^T\hat{A}^T$$

Adjoint/Hermitian conjugate

Given a matrix $\hat{A}$, the adjoint of $\hat{A}$ is

$$\hat{A}^\dagger = (\hat{A}^*)^T$$

$$= (\hat{A}^*_{ij})^T$$

$$= \hat{A}^*_{ji}$$

Because of the transpose part, we have

$$(\hat{A}\hat{B}\hat{C}\cdots\hat{Z})^\dagger = \hat{Z}^\dagger\dots\hat{C}^\dagger\hat{B}^\dagger\hat{A}^\dagger$$

The trace of a matrix

Given a matrix $\hat{A}$, the trace of $\hat{A}$ is the sum of the diagonal elements of $\hat{A}$:

$$\mathrm{Tr}(\hat{A}) = A_{11} + A_{22} + A_{33} + \dots + A_{NN}$$

$$= \sum_{n=1}^{N} A_{nn}$$

One can readily show that

$$\mathrm{Tr}(\hat{A}\pm\hat{B}) = \mathrm{Tr}(\hat{A}) \pm \mathrm{Tr}(\hat{B})$$

$$\mathrm{Tr}(\hat{A}^T) = \mathrm{Tr}(\hat{A})$$

$$\mathrm{Tr}(\hat{A}^\dagger) = [\mathrm{Tr}(\hat{A})]^*$$

More importantly,

$$\mathrm{Tr}(\hat{A}\hat{B}) = \mathrm{Tr}(\hat{B}\hat{A}) \text{ and}$$

$$\mathrm{Tr}(\hat{A}\hat{B}\hat{C}) = \mathrm{Tr}(\hat{B}\hat{C}\hat{A}) = \mathrm{Tr}(\hat{C}\hat{A}\hat{B})$$

Traceless matrices

A matrix which is constructed from the commutator of two matrices is always traceless.

$$\hat{C} = [\hat{A},\hat{B}]$$

$$\mathrm{Tr}(\hat{C}) = \mathrm{Tr}([\hat{A},\hat{B}])$$

$$= \mathrm{Tr}(\hat{A}\hat{B} - \hat{B}\hat{A})$$

$$= \mathrm{Tr}(\hat{A}\hat{B}) - \mathrm{Tr}(\hat{B}\hat{A})$$

$$= \mathrm{Tr}(\hat{A}\hat{B}) - \mathrm{Tr}(\hat{A}\hat{B})$$

$$= 0$$

finite dimensional