Derivative of Unitary is not always -iHU

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Abstract

$i\dot{U} = HU$ (or $\dot{U} = -iHU$) is the equation that is said to govern the evolution of a unitary matrix U given the Hamiltonian H of the system. This equation is said to hold true even if the Hamiltonian is time dependent. We show iU = HU (or $\dot{U} = -iHU$) is the equation that is said to govern the evolution of a unitary matrix U given the Hamiltonian H of the system. This equation is said to hold true even if the Hamiltonian is time dependent. We show in this paper that $i\dot{U} = HU$ may not always hold for time dependent Hamiltonians.this paper that $i\dot{U} = HU$ may not always hold for time dependent Hamiltonians.

Introduction

The evolution of a unitary operator is given by $i\dot{U} = HU$. (where H is the Hamiltonian of the system). This equation is so common place that no one bothers to cite it. It is considered as a standard part of the curricula of certain courses, in physics books (see [1]) and even in allied engineering fields. For example see [2] (a course in Nuclear Engineering). Needless to say, the formula also has been extensively used in the literature. For example see Equation 35 in [3], Equation 25 in [4], Equation 7 in [5], Equation 4 in [6].

The organisation of next section is as follows:
In subsection A we show that for any matrix A, $[A, \dot{A}]$ is not necessarily equal to $\mathbf{0}$. Subsection B deals with the derivative of e^A. From this we find the derivative of a unitary matrix in subsection C. We show in subsection D as to why in case of time independent Hamiltonian $i\dot{U} = HU$ more or less holds good.

Finally in section III, we synthesize the various lines of argument into a concluding paragraph.

Proof

A and its time derivative don't commute

The title can be mathematically paraphrased as

$[A, \dot{A}] \neq \mathbf{0}$. For any function $f(A)$ (matrix or scalar valued) $\dot{f} = \frac{\partial f}{\partial t}$. Say we have a matrix valued function

$$A(t) = \begin{bmatrix} a & b \\ c & d \end{bmatrix} \tag{1}$$

where a,b,c,d are four distinct functions of time. We can differentiate $A(t)$ as follows [7], [8]

$$\dot{A} = \begin{bmatrix} \dot{a} & \dot{b} \\ \dot{c} & \dot{d} \end{bmatrix} \tag{2}$$

Thus,

$$\begin{aligned} \left[A, \dot{A}\right] &= A\dot{A} - \dot{A}A \\ &= \begin{bmatrix} a & b \\ c & d \end{bmatrix} \begin{bmatrix} \dot{a} & \dot{b} \\ \dot{c} & \dot{d} \end{bmatrix} - \begin{bmatrix} \dot{a} & \dot{b} \\ \dot{c} & \dot{d} \end{bmatrix} \begin{bmatrix} a & b \\ c & d \end{bmatrix} \\ &= \begin{bmatrix} b\dot{c} - \dot{b}c & a\dot{b} - \dot{a}b + b\dot{d} - \dot{b}d \\ c\dot{a} - \dot{c}a + d\dot{c} - \dot{d}c & -\left(b\dot{c} - \dot{b}c\right) \end{bmatrix} \end{aligned} \tag{3}$$

Any of the elements of $\left[A, \dot{A}\right]$ are not necessarily zero at all times. Thus $\left[A, \dot{A}\right]$ is not necessarily zero. Special cases where $\left[A, \dot{A}\right] = \mathbf{0}$

1. A is a constant function. This makes $\dot{A} = \mathbf{0}$. Because of this $\left[A, \dot{A}\right] = \mathbf{0}$
2. $A = \lambda(t)I \Rightarrow \dot{A} = \dot{\lambda}(t)I$

$$\begin{aligned} \therefore \left[A, \dot{A}\right] &= A\dot{A} - \dot{A}A \\ &= (\lambda I)\left(\dot{\lambda} I\right) - \left(\dot{\lambda} I\right)(\lambda I) \\ &= \left(\lambda\dot{\lambda} I\right) - \left(\dot{\lambda}\lambda I\right) \\ &= \mathbf{0} \end{aligned} \tag{4}$$

3. A is a diagonal matrix. This implies that $b, c = 0$. From Equation 3 we have $\left[A, \dot{A}\right] = \mathbf{0}$.
4. $A = tB$, where B is a constant matrix.

$$\begin{aligned} \therefore \left[A, \dot{A}\right] &= A\dot{A} - \dot{A}A \\ &= tBB - BtB \\ &= \mathbf{0} \end{aligned} \tag{5}$$

It can be easily shown that even if A is a skew Hermitian $\left[A, \dot{A}\right]$ is not necessarily zero. For the rest of discussion we only consider A such that $\left[A, \dot{A}\right] \neq \mathbf{0} \, \forall \, t$

In the case $\left[A, \dot{A}\right] = \mathbf{0}$, everything is true and wonderful.

Derivative of matrix exponential functions

Let us see what we get on differentiating A^2. From the product rule, we have

$$(\dot{A^2}) = A\dot{A} + \dot{A}A \tag{6}$$

But, given the previous discussion

$$\begin{aligned}(\dot{A^2}) &\neq \dot{A}A + \dot{A}A \left(\because \left[A, \dot{A}\right] \neq 0\right) \\ &\neq 2\dot{A}A\end{aligned} \tag{7}$$

Similarly,

$$(\dot{A^3}) \neq 3\dot{A}A \tag{8}$$

Instead, we obtain

$$(\dot{A^3}) = AA\dot{A} + A\dot{A}A + \dot{A}AA \tag{9}$$

For A^n, we get

$$(\dot{A^n}) = (A\dot{A^{n-1}}) \tag{10}$$

$$= A(\dot{A^{n-1}}) + \dot{A}A^{n-1} \tag{11}$$

Continuing down, we are left with

$$(\dot{A^n}) = \sum_{m=0}^{n-1} A^m \dot{A} A^{n-(m+1)} \tag{12}$$

We know that

$$e^A = \sum_{n=0}^{\infty} \frac{A^n}{n!} \tag{13}$$

On applying the above train of thought

$$(\dot{e^A}) = \sum_{n=0}^{\infty} \sum_{m=0}^{n-1} \frac{A^m \dot{A} A^{n-(m+1)}}{n!} \tag{14}$$

[9] and [10] have rewritten the above formula in a more pleasing format. The simplified form of Equation 2.1 from [10] in terms of our notation is as follows

$$(\dot{e^A}) = \int_0^1 e^{A(1-s)} \dot{A} e^{As} ds \tag{15}$$

Let us try to derive Equation 15 from Equation 14. The steps below are inspired from [9].
When we differentiate A^n we obtain a series in which each term is a permutation of a product of $n-1$ $A's$ and one $\dot{A}$. So the series in Equation 14 can be rewritten as:

$$(\dot{e^A}) = \sum_{p=0}^{\infty}\sum_{m=0}^{\infty} \frac{A^m \dot{A} A^p}{(m+p+1)!} \;\; (\because n = m+p+1) \tag{16}$$

$$= \sum_{p=0}^{\infty}\sum_{m=0}^{\infty} \frac{A^m \dot{A} A^p}{m!\,p!} \frac{m!\,p!}{(m+p+1)!} \tag{17}$$

We know that

$$\int_0^1 (1-s)^m s^p ds = \frac{m!p!}{(m+p+1)!} \tag{18}$$

Hence:

$$(\dot{e^A}) = \sum_{p=0}^{\infty}\sum_{m=0}^{\infty} \frac{A^m \dot{A} A^p}{m!\,p!} \int_0^1 (1-s)^m s^p ds \tag{19}$$

$$(\dot{e^A}) = \int_0^1 \sum_{p=0}^{\infty}\sum_{m=0}^{\infty} \frac{(1-s)^m A^m \dot{A} A^p s^p}{m!\,p!} ds \tag{20}$$

$$(\dot{e^A}) = \int_0^1 \sum_{p=0}^{\infty} \left(\sum_{m=0}^{\infty} \frac{(1-s)^m A^m}{m!} \right) \dot{A} \frac{A^p s^p}{p!} ds \tag{21}$$

$$(\dot{e^A}) = \int_0^1 \sum_{p=0}^{\infty} e^{(1-s)A} \dot{A} \frac{A^p s^p}{p!} ds \tag{22}$$

$$(\dot{e^A}) = \int_0^1 e^{(1-s)A} \dot{A}\, e^{As}\, ds \tag{23}$$

Since, $\left[A, \dot{A}\right] \neq \mathbf{0}$, $\left[e^A, \dot{A}\right] \neq \mathbf{0}$. Given that $\left[e^A, \dot{A}\right] \neq \mathbf{0}$, we can say that

$$e^{A(1-s)} \dot{A} e^{As} \neq \dot{A} e^{A(1-s)} e^{As} \tag{24}$$
$$\neq \dot{A} e^A$$

Hence,

$$(\dot{e^A}) \neq \int_0^1 \dot{A} e^A ds$$
$$(\dot{e^A}) \neq \dot{A} e^A \tag{25}$$

From Equation 15, 24 and 25 one can safely say that $(\dot{e^A})$ *can not be* written as Be^A (where $B = g(\dot{A})$ i.e B is a function of only $\dot{A}$).

Derivative of a unitary matrix

We can write $U = e^{\Omega(t)}$, where $\Omega(t)$ is a matrix valued function of time. By the virtue of its construction, $\Omega(t)$ is an skew Hermitian matrix. Thus from end of section , $\left[\Omega, \dot{\Omega}\right] \neq \mathbf{0}$

Since $(\dot{e^A}) \neq B(\dot{A})e^A$ as proved in end of section

$$\dot{U} \neq B(\dot{\Omega})e^{\Omega} \qquad \text{or}$$
$$\dot{U} \neq B(\dot{\Omega})U \tag{26}$$

In words it means that $\dot{U}$ cannot be written as a product of function of $B(\dot{\Omega})$ and U. We know that for time independent Hamiltonians $U = e^{-iHt}$. So it is fair to assume that Ω may depend on the Hamiltonian H in some way. Since Ω depends on the Hamiltonian H , $\dot{\boldsymbol{\Omega}}$ too is a function of H .

$\therefore$ From the previous Equation 26

$$\dot{U} \neq B'(H)U \tag{27}$$

where B' is another function only of H such that $B'(H) = B(\dot{\Omega})$.

Taking things a step further $\dot{U} \neq -iHU$ for time dependent Hamiltonians.

Time independent Hamiltonians

The rule $\dot{U} = -iHU$ still holds good for time independent Hamiltonians, but here too things are not the same as before. From special case 1 from subsection we have

$$\left[H, \dot{H}\right] = \mathbf{0} \qquad \text{since } H \text{ is time independent} \tag{28}$$

From the discussion in sub-section we can say that

$$\left[H, e^{-iHt}\right] = \mathbf{0} \tag{29}$$
$$[H, U] = \mathbf{0} \tag{30}$$

Thus $\dot{U} = -iHU$ can be transformed to $\dot{U} = -iUH$. So The order of U, H does not really matter on the right hand side the equation $\dot{U} = -iHU$ for time independent Hamiltonians.

Conclusion

In this paper, we have shown that $\dot{U}$ is not always equal to $-iHU$ for time dependant Hamiltonians. This does not mean that it is not possible. One of the ways it may be possible is that the functions a, b, c, d of A align themselves in such a way that $\left[A, \dot{A}\right] = \mathbf{0}$ (other than those special cases considered in section). Under *more severely* restrictive conditions than those considered here, [12], [13] have shown that $(\dot{e^A}) = \dot{A}e^A$, even if $\left[A, \dot{A}\right] \neq \mathbf{0}$. But these restrictions coupled with the Hermiticity requirements of the Hamiltonian make this very unlikely to happen.

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