The time evolution operator as a time-ordered exponential

1. The time evolution operator and its properties

The time evolution of a state vector in the quantum mechanical Hilbert space is governed by the Schrodinger equation,

$$i\hbar\frac{d}{dt}\left|\psi(t)\right\rangle = H(t)\left|\psi(t)\right\rangle \,, \tag{1}$$

where $H(t)$ is the Hamiltonian operator (which may depend on the time t). The solution to this equation defines the time evolution operator, $U(t, t_0)$,

$$\left|\psi(t)\right\rangle = U(t,t_0)\left|\psi(t_0)\right\rangle \,, \tag{2}$$

where the state vector at time t_0 provides the initial condition for the time evolution of $\left|\psi(t)\right\rangle$. Note that

$$U(t,t) = I \,, \tag{3}$$

where I is the identity operator. In addition, by applying eq. (2) twice, one easily obtains,

$$U(t_2,t_0) = U(t_2,t_1)U(t_1,t_0)\,. \tag{4}$$

Plugging in eq. (2) into eq. (1) yields a partial differential equation for $U(t, t_0)$,

$$\left\{i\hbar\frac{\partial}{\partial t} - H(t)\right\}U(t,t_0)\left|\psi(t_0)\right\rangle = 0\,.$$

Since $\left|\psi(t_0)\right\rangle$ is arbitrary, it follows that $U(t, t_0)$ must satisfy,

$$i\hbar\frac{\partial}{\partial t}U(t,t_0) = H(t)U(t,t_0)\,, \tag{5}$$

subject to the initial condition, $U(t_0, t_0) = I$.

The goal of these notes is to solve the differential equation [eq. (5)] for $U(t, t_0)$. First, we will derive an expression for $U(t + \delta t, t)$ in the limit of $\delta t \to 0$. By Taylor expansion,

$$U(t+\delta t,t_0) = U(t,t_0) + \delta t\frac{\partial U}{\partial t}(t,t_0) + \mathcal{O}\big((\delta t)^2\big)\,,$$

where we discard terms that are quadratic in the infinitesimal quantity δt. Using eq. (5), it follows that

$$U(t+\delta t,t_0) = U(t,t_0) - \frac{i}{\hbar}H(t)U(t,t_0)\delta t + \mathcal{O}\big((\delta t)^2\big)\,.$$

Finally, we can set $t_0 = t$ and make use of eq. (3) to obtain the final result,

$$U(t+\delta t, t) = I - \frac{i}{\hbar} H(t)\delta t + \mathcal{O}\big((\delta t)^2\big)\,. \tag{6}$$

Note that an alternative expression for eq. (6) is,

$$U(t+\delta t, t) = \exp\big\{-iH(t)\delta t/\hbar\big\} + \mathcal{O}\big((\delta t)^2\big)\,, \tag{7}$$

since the expressions exhibited in eqs. (6) and (7) differ only in the terms of $\mathcal{O}\big((\delta t)^2\big)$.

2. An explicit formula for the time evolution operator–Case 1: $\big[\boldsymbol{H(t_i)}, \boldsymbol{H(t_j)}\big] = \mathbf{0}$

To obtain an explicit formula for the time evolution operator, let us divide up he time axis from t_0 to t in N equal subintervals, each one of length

$$\varepsilon \equiv \frac{t - t_0}{N}\,. \tag{8}$$

If we repeatedly apply eq. (4), it follows that

$$U(t, t_0) = \prod_{k=1}^{N} U\big(t_0 + k\varepsilon\,,\, t_0 + (k-1)\varepsilon\big)\,. \tag{9}$$

Using eq. (7) and working to first order in ε,

$$U\big(t_0 + k\varepsilon\,,\, t_0 + (k-1)\varepsilon\big) \simeq \exp\left\{-\frac{i\varepsilon}{\hbar} H\big(t_0 + (k-1)\varepsilon\big)\right\}\,. \tag{10}$$

Hence, if we take the limit of $N \to \infty$, or equivalently $\varepsilon \to 0$, eq. (9) yields,

$$\begin{aligned} U(t, t_0) &= \lim_{\varepsilon \to 0} \prod_{k=1}^{N} \exp\left\{-\frac{i\varepsilon}{\hbar} H\big(t_0 + (k-1)\varepsilon\big)\right\} \\ &= \lim_{\varepsilon \to 0} \exp\left\{-\frac{i\varepsilon}{\hbar} H\big(t_0\big)\right\} \exp\left\{-\frac{i\varepsilon}{\hbar} H\big(t_0 + \varepsilon\big)\right\} \cdots \exp\left\{-\frac{i\varepsilon}{\hbar} H\big(t - \varepsilon\big)\right\}\,. \end{aligned} \tag{11}$$

At this point in the calculation, we would like to combine all of the exponentials in eq. (11). However, the $H(t_i)$ are operators and in general, $H(t_i)$ ahd $H(t_j)$ do not commute if $i \neq j$. In this case it is impractical to evaluate eq. (11) further. Indeed, if $\big[A, B\big] \neq 0$, then the Baker-Campbell-Hausdorff formula yields an extremely complicated expression,

$$\exp A \exp B = \exp\big\{A + B + \tfrac{1}{2}[A, B\big] + \cdots\big\}\,,$$

where the $\cdots$ indicates an infinite series of nested commutators. To try to apply this to eq. (11) looks quite hopeless.

Thus, in this section, we shall first assume that the Hamiltonian operator satisfies,

$$\big[H(t_i), H(t_j)\big] = 0\,, \tag{12}$$

for all choices of t_i and t_j. In this case, we can simplify eq. (11),

$$U(t,t_0) = \lim_{\varepsilon\to 0} \exp\left\{-\frac{i\varepsilon}{\hbar}\sum_{k=0}^{N-1} H\big(t_0+k\varepsilon\big)\right\} \tag{13}$$

Since $\varepsilon = (t-t_0)/N$, it follows that $N\to\infty$ and $t_0+(N-1)\varepsilon \to t$ as $\varepsilon\to 0$. Hence,

$$\lim_{\varepsilon\to 0}\varepsilon\sum_{k=0}^{N-1} H\big(t_0+k\varepsilon\big) = \int_{t_0}^{t} H(t)\,dt\,. \tag{14}$$

Consequently, eq. (13) yields,

$$\boxed{U(t,t_0) = \exp\left\{-\frac{i}{\hbar}\int_{t_0}^{t} H(t)\,dt\right\}\,, \qquad \text{if } \big[H(t_i), H(t_j)\big] = 0.} \tag{15}$$

As usual, the exponential of an operator is defined via its Taylor series.

A special case of eq. (15) is the case of a time-independent Hamiltonian. In this case, eq. (12) is trivially satisfied, and

$$\int_{t_0}^{t} H\,dt = H\int_{t_0}^{t} dt = H(t-t_0)\,.$$

Inserting this result into eq. (15) yields

$$\boxed{U(t,t_0) = e^{-iH(t-t_0)/\hbar}\,, \qquad \text{if } H \text{ is time-independent.}} \tag{16}$$

Indeed, one can derive eq. (15) directly from eq. (5) by writing

$$\left[\frac{\partial}{\partial t}U(t,t_0)\right]U^{-1}(t,t_0) = -\frac{i}{\hbar}H(t)\,. \tag{17}$$

In order to proceed, we would like to write,

$$\frac{\partial}{\partial t}\ln U(t,t_0) = \left[\frac{\partial}{\partial t}U(t,t_0)\right]U^{-1}(t,t_0)\,. \tag{18}$$

In general, eq. (18) is not true unless U and $\partial U/\partial t$ commute (see Appendix A), in which case one is free to place the factor of U^{-1} in eq. (18) to the left or to the right of $\partial U/\partial t$. If we assume that eq. (18) holds, then it follows that

$$\frac{\partial}{\partial t}\ln U(t,t_0) = -\frac{i}{\hbar}H(t)\,.$$

Integrating this equation form t_0 to t and imposing the initial condition, $U(t_0,t_0) = I$, yields

$$\ln U(t,t_0) = -\frac{i}{\hbar}\int_{t_0}^{t} H(t)\,dt\,, \tag{19}$$

which when exponentiated yields eq. (15). In particular, if $\big[H(t_i), H(t_j)\big] = 0$, then the expression for $U(t,t_0)$ given by eq. (15) implies that U and $\partial U/\partial t$ commute, in which case the use of eq. (18) in obtaining eq. (19) is justified.

3. An explicit formula for the time evolution operator–Case 2: $\big[H(t_i), H(t_j)\big] \neq 0$

In the case of $\big[H(t_i), H(t_j)\big] \neq 0$ it is not practical to employ eq. (11). Hence, we will make use of another technique. Given the differential equation of eq. (5), with the initial condition $U(t_0, t_0) = I$, it is possible to rewrite this as an integral equation,

$$U(t, t_0) = I - \frac{i}{\hbar}\int_{t_0}^{t} H(t')U(t', t_0)\, dt' \,. \tag{20}$$

There are two points worth noting. First, the initial condition $U(t_0, t_0) = I$ is automatically incorporated into the integral equation given in eq. (20) since the integral on the right hand side of eq. (20) vanishes when $t = t_0$. Second, eq. (20) does not immediately provide the solution for $U(t, t_0)$ since $U(t, t_0)$ appears both on the left hand side and the right hand side of eq. (20). To show that eq. (20) is equivalent to eq. (5) subject to the initial condition $U(t_0, t_0) = I$, we simply note that the fundamental theorem of calculus implies that

$$\frac{\partial}{\partial t}\int_{t_0}^{t} H(t')U(t', t_0)\, dt' = H(t)U(t, t_0)\,.$$

Hence, taking the partial derivative of eq. (20) with respect to t immediately yields eq. (5).

We can solve eq. (20) by an iterative procedure. To make the procedure clear, I shall replace eq. (20) with

$$U(t, t_0) = I - \frac{ia}{\hbar}\int_{t_0}^{t} H(t')U(t', t_0)\, dt' \,, \tag{21}$$

where a is a real positive parameter. The parameter a is being used for "bookkeeping" (sometimes called a bookkeeping parameter in the physics literature). At the end of the calculation, we can set $a = 1$ to regain eq. (20).

The iterative procedure consists of obtaining better and better approximations for $U(t, t_0)$ by working to $\mathcal{O}(a^N)$ for $N = 1, 2, 3, \ldots$. At step one, we approximate $U(t', t_0) = I$ on the right hand side of eq. (21), which yields an expression for $U(t, t_0)$ [denoted below by $U_1(t, t_0)$] that is valid to $\mathcal{O}(a)$,

$$U_1(t, t_0) = I - \frac{ia}{\hbar}\int_{t_0}^{t} H(t'')\, dt'' \,,$$

where we have called the integration variable t'' for later convenience. At step two, we approximate $U(t, t_0) = U_1(t, t_0)$ on the right hand side of eq. (21), which yields an expression for $U(t, t_0)$ [denoted below by $U_2(t, t_0)$] that is valid to $\mathcal{O}(a^2)$,

$$U_2(t, t_0) = I - \frac{ia}{\hbar}\int_{t_0}^{t} H(t')\, dt' + \left(\frac{ia}{\hbar}\right)^2 \int_{t_0}^{t} H(t')\, dt' \int_{t_0}^{t'} H(t'')dt'' \,.$$

It should be clear how to carry the iterative procedure through N steps.

$$U_N(t, t_0) = I + \sum_{n=1}^{N}\left(-\frac{ia}{\hbar}\right)^n \int_{t_0}^{t} dt_1 \int_{t_0}^{t_1} dt_2 \cdots \int_{t_0}^{t_{n-1}} dt_n\, H(t_1)H(t_2)\cdots H(t_n)\,,$$

where we have employed as integrating variables t_1, $t_2, \ldots t_n$ instead of the more awkward t', t'', ...

I now assert the following. $U_N(t,t_0)$ becomes a better and better approximation to $U(t,t_0)$ as N gets larger. If we formally take the limit of $N\to\infty$, we should end up with the exact solution,

$$U(t,t_0)=I+\sum_{n=1}^{\infty}\left(-\frac{ia}{\hbar}\right)^n\int_{t_0}^{t}dt_1\int_{t_0}^{t_1}dt_2\cdots\int_{t_0}^{t_{n-1}}dt_n\,H(t_1)H(t_2)\cdots H(t_n)\,,$$

under the assumption that the infinite series converges.[1] Finally, setting the bookkeeping parameter $a=1$, we have our final result,

$$\boxed{U(t,t_0)=I+\sum_{n=1}^{\infty}\left(-\frac{i}{\hbar}\right)^n\int_{t_0}^{t}dt_1\int_{t_0}^{t_1}dt_2\cdots\int_{t_0}^{t_{n-1}}dt_n\,H(t_1)H(t_2)\cdots H(t_n)\,,}\qquad(22)$$

which is sometimes known as the *Dyson series*. Truncating the sum in eq. (22) yields approximate expressions for $U(t,t_0)$, which is the basis for time-dependent perturbation theory that will be treated in Physics 216.

4. The time-ordered exponential

At this stage, it is not obvious that eq. (22) reduces to eq. (15) if $\big[H(t_i),H(t_j)\big]=0$. In particular, the integration limits in the integral over t_n involves t_{n-1}, etc in the n-fold integral that appears in eq. (22) . This does not occur if one performs a Taylor series of the exponential in eq. (15). Thus, the goal of this section is to find a way to rewrite the n-fold integral in eq. (22) such that the integration regions do not depend of the integration variables, but instead simply go from t_0 to t in all n integrations!

To achieve the stated goal, one must introduce the *time-ordered product* of operators,

$$T\big[H(t_1)H(t_2)\cdots H(t_n)\big]=H(t_{i_1})H(t_{i_2})\cdots H(t_{i_n})\,,\quad\text{where } t_{i_1}>t_{i_2}>\cdots>t_{i_n},\qquad(23)$$

and n is a positive integer.[2] That is, the time-ordered product of operators is an instruction to reorder the operators such that the time arguments of the corresponding operators *decrease* as one moves from the left to the right. For example, the largest time appears in the argument of the first operator and the smallest time appears in the argument of the last operator. Note that if any of the time arguments in eq. (23) coincide, this does not cause any problem since $H(t)$ commutes with itself.

Using the time-ordered product, we can rewrite the nth term of eq. (22) in a more convenient form in which the integration limits are uncoupled. It is instructive to see how this is accomplished for the $n=2$ term of the series (with the general proof for the nth term in the series left to the reader).

[1] It is highly nontrivial to prove that the infinite series converges. In some cases, the best we can hope for is that the series is an asymptotic series representation of $U(t,t_0)$.

[2] If $n=1$, then we simply define $T\big[H(t)\big]=H(t)$. For $n\geq 2$, the ordering of the operators specified on the right hand side of eq. (23) matters if the Hamiltonian operators evaluated at different times do not commute. On the other hand, if $\big[H(t_i),H(t_j)\big]=0$, then the T symbol has no effect.

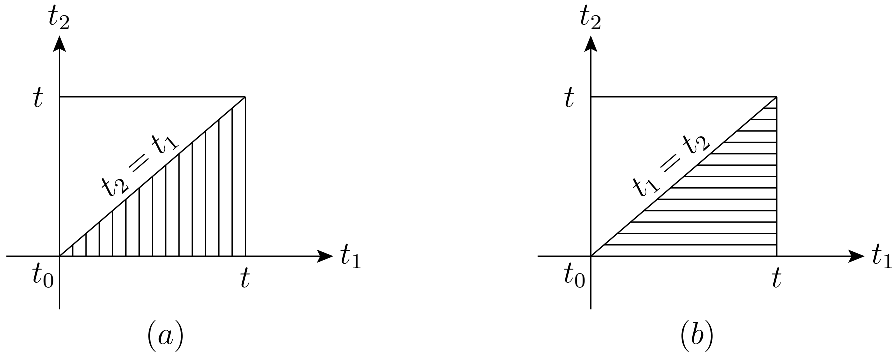

Figure 1: (a) The integration region, $t_0 \leq t_1 \leq t$ and $t_0 \leq t_2 \leq t_1$, employed in eq. (24). (b) The integration region, $t_0 \leq t_2 \leq t$ and $t_2 \leq t_1 \leq t$, employed in eq. (25) after interchanging the order of integration .

Consider the integral J_2,

$$J_2 \equiv \int_{t_0}^{t} dt_1 \int_{t_0}^{t_1} dt_2\, H(t_1)H(t_2) = \int_{t_0}^{t} dt_1 \int_{t_0}^{t_1} dt_2\, T\big[H(t_1)H(t_2)\big]\,. \tag{24}$$

The region defined by $0 \leq t_1, t_2 \leq t$ is an area bounded by a square. The integration region in eq. (24), exhibited in Figure 1(a), consists of the area bounded by half of the square where $t_2 \leq t_1$, which allows us to insert the T symbol in the second integral above. That is, $T\big[H(t_1)H(t_2)\big] = H(t_1)H(t_2)$ in the region where $t_2 \leq t_1$.

One can also evaluate J_2 by interchanging the order of integration, in which case the new region of integration is exhibited in Figure 1(b). The value of the integral does not change, so that

$$J_2 = \int_{t_0}^{t} dt_1 \int_{t_0}^{t_1} dt_2\, H(t_1)H(t_2) = \int_{t_0}^{t} dt_2 \int_{t_2}^{t} dt_1\, H(t_1)H(t_2)\,. \tag{25}$$

Since the integration variables, t_1 and t_2, are dummy labels, one can relabel the integration variables in the last integral of eq. (25) by $t_1 \to t_2$ and $t_2 \to t_1$, which yields

$$J_2 = \int_{t_0}^{t} dt_1 \int_{t_1}^{t} dt_2\, H(t_2)H(t_1) = \int_{t_0}^{t} dt_1 \int_{t_1}^{t} dt_2\, T\big[H(t_1)H(t_2)\big]\,. \tag{26}$$

We are allowed to insert the T symbol in the second integral above since $t_2 \geq t_1$, in which case $T\big[H(t_1)H(t_2)\big] = H(t_2)H(t_1)$. That is, the integration region now consists of the area of the half square *above* the diagonal line shown in Figure 1(a).

Consequently, we now have two different expressions for J_2,

$$J_2 = \int_{t_0}^{t} dt_1 \int_{t_0}^{t_1} dt_2\, T\big[H(t_1)H(t_2)\big] = \int_{t_0}^{t} dt_1 \int_{t_1}^{t} dt_2\, T\big[H(t_1)H(t_2)\big]\,. \tag{27}$$

Therefore, $2J_2$ is equal to the sum of the two integrals given in eq. (27). By adding the two integrals, the dependence on the integration limit t_1 disappears. The integration region is now the area bounded by the full square, i.e. $0 \leq t_1, t_2 \leq t$. After dividing by two, we end up with,

$$J_2 = \frac{1}{2}\int_{t_0}^{t} dt_1 \int_{t_0}^{t} dt_2\, T\big[H(t_1)H(t_2)\big]\,. \tag{28}$$

Remarkably, the integration limits are now decoupled!

It should now be clear how this works in the case of the nth term of the series in eq. (22). The original integration region of the integral J_n consists of the hyper-volume bounded by the hypercube defined by $0 \leq t_1, t_2, \ldots, t_n \leq t$ such that $t_1 \geq t_2 \geq t_3 \cdots \geq t_n$. This region is a fraction $1/n!$ of the hypercube. By interchanging the order of integration in $n! - 1$ possible ways and then appropriately relabeling the integration variables, one obtains alternative expressions for J_n that cover the remaining $n! - 1$ regions of the hypercube. The end result is an integral over the entire hypercube, $0 \leq t_1, t_2, \ldots, t_n \leq t$ (with the integration limits decoupled),

$$\begin{aligned} J_n &\equiv \int_{t_0}^{t} dt_1 \int_{t_0}^{t_1} dt_2 \cdots \int_{t_0}^{t_{n-1}} dt_n \, H(t_1)H(t_2)\cdots H(t_n) \\ &= \frac{1}{n!} \int_{t_0}^{t} dt_1 \int_{t_0}^{t} dt_2 \cdots \int_{t_0}^{t} dt_n \, T\big[H(t_1)H(t_2)\cdots H(t_n)\big] \,. \end{aligned} \tag{29}$$

Employing this result in eq. (22), we arrive at our final result,

$$U(t, t_0) = I + \sum_{n=1}^{\infty} \frac{1}{n!} \left(-\frac{i}{\hbar}\right)^n \int_{t_0}^{t} dt_1 \int_{t_0}^{t} dt_2 \cdots \int_{t_0}^{t} dt_n \, T\big[H(t_1)H(t_2)\cdots H(t_n)\big] \,. \tag{30}$$

Using eq. (30), we now see how to recover eq. (22) when $\big[H(t_i), H(t_j)\big] = 0$. In this case, the T symbol in eq. (30) is redundant, since we are free to reorder the individual operators. Hence, it follows that if $\big[H(t_i), H(t_j)\big] = 0$, then

$$\begin{aligned} U(t, t_0) &= I + \sum_{n=1}^{\infty} \frac{1}{n!} \left(-\frac{i}{\hbar}\right)^n \int_{t_0}^{t} dt_1 \int_{t_0}^{t} dt_2 \cdots \int_{t_0}^{t} dt_n \, H(t_1)H(t_2)\cdots H(t_n) \\ &= I + \sum_{n=1}^{\infty} \frac{1}{n!} \left(-\frac{i}{\hbar}\right)^n \left(\int_{t_0}^{t} H(t')\, dt'\right)^n = \exp\left\{-\frac{i}{\hbar}\int_{t_0}^{t} H(t)\, dt\right\} \,, \end{aligned} \tag{31}$$

after using the Taylor series definition of the exponential.

Comparing eqs. (30) and (31), we are motivated to introduce the *time-ordered exponential*, $T\exp$, which is defined by the following expression,

$$T\exp\left\{-\frac{i}{\hbar}\int_{t_0}^{t} H(t)\, dt\right\} \equiv I + \sum_{n=1}^{\infty} \frac{1}{n!} \left(-\frac{i}{\hbar}\right)^n \int_{t_0}^{t} dt_1 \int_{t_0}^{t} dt_2 \cdots \int_{t_0}^{t} dt_n \, T\big[H(t_1)H(t_2)\cdots H(t_n)\big] \,. \tag{32}$$

Thus, in light of eqs. (30) and (32), we conclude that the most general solution to

$$i\hbar \frac{\partial}{\partial t} U(t, t_0) = H(t) U(t, t_0) \,, \tag{33}$$

subject to the initial condition, $U(t_0, t_0) = I$, is given by

$$\boxed{U(t, t_0) = T\exp\left\{-\frac{i}{\hbar}\int_{t_0}^{t} H(t)\, dt\right\} \,.} \tag{34}$$

Of course, the remarkably simple form of eq. (34) hides the complexity that is contained in the definition of the time-ordered exponential given in eq. (32). Nevertheless, it provides a very useful shorthand notation to use in the case where $\big[H(t_i), H(t_j)\big] \neq 0$. As noted above, if the Hamiltonian operators evaluated at different times commute, then we may simply drop the T symbol, since it has no effect in this case.

The differential equation given in eq. (33) arises in many different circumstances in mathematical physics. In some of these circumstances, the parameter t has nothing to do with time. But, as long as non-commuting operators are involved, the solution to eq. (33) can be written as a T-ordered exponential, where the T ordering is defined in a way analogous to that of eq. (23).

Appendix A: Formula for the derivative of $\ln A(t)$ where A is a linear operator

Start with the following formula (whose derivation is left to the reader),

$$\ln(A+B) - \ln A = \int_0^\infty du \left\{ \big(A+uI\big)^{-1} - \big(A+B+uI\big)^{-1} \right\}, \tag{35}$$

Assume that the operator A depends on a parameter t. Using the definition of the derivative,

$$\frac{d}{dt}\ln A(t) = \lim_{h\to 0} \frac{\ln(A(t+h) - \ln A(t)}{h} = \lim_{h\to 0} \frac{\ln\big[A(t) + h dA/dt + \mathcal{O}(h^2)\big] - \ln A(t)}{h}\,.$$

Denoting $B = h dA/dt$ and making use of eq. (35),

$$\frac{d}{dt}\ln A(t) = \lim_{h\to 0} \frac{1}{h}\int_0^\infty du \left\{ \big(A+uI\big)^{-1} - \big(A+hdA/dt+uI\big)^{-1} \right\}, \tag{36}$$

For an infinitesimal h, we have

$$\begin{aligned}
\big(A+hdA/dt+uI\big)^{-1} &= \big[(A+uI)(I+h(A+uI)^{-1}dA/dt)\big]^{-1} \\
&= (I+h(A+uI)^{-1}dA/dt)^{-1}(A+uI)^{-1} \\
&= (I-h(A+uI)^{-1}dA/dt)(A+uI)^{-1} + \mathcal{O}(h^2) \\
&= (A+uI)^{-1} - h(A+uI)^{-1}dA/dt(A+uI)^{-1} + \mathcal{O}(h^2)\,.
\end{aligned} \tag{37}$$

Inserting this result into eq. (36) yields

$$\frac{d}{dt}\ln A(t) = \int_0^\infty du\,(A+uI)^{-1}\frac{dA}{dt}(A+uI)^{-1}\,. \tag{38}$$

Finally, if we change variables using $u = (1-s)/s$, one obtains an alternative form,

$$\frac{d}{dt}\ln A(t) = \int_0^1 ds\,\big[sA+(1-s)I\big]^{-1}\frac{dA}{dt}\big[sA+(1-s)I\big]^{-1}\,. \tag{39}$$

One can check that if $[A, dA/dt] = 0$, then eq. (38) [or eq. (39)] reduces to,

$$\frac{d}{dt}\ln A(t) = A^{-1}\frac{dA}{dt} = \frac{dA}{dt}A^{-1}\,.$$