Optimal Control of a Spin System Acting on a Single Quantum Bit

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Abstract: We study a quantum spin system acting on a single quantum bit. The evolution of this system is governed by the Schrödinger equation which takes the form of a right-invariant system on the special unitary group SU(2)with two control inputs. Using a suitable version of Pontryagin's Principle which is tailor-made for control problems on Lie groups, the optimal controls are derived in two cases: the energy-optimal case (in which the control effort is minimized for a specified end time) and the time-optimal case (in which the control duration is minimized for given constraints on the size of the controls).

Key-Words: Nonlinear control, optimal control, quantum spin systems.

1 Problem Formulation

The evolution of the spin system we want to consider is given by the Schrödinger equation

$$\dot{U}(t) = (c(t)A + u(t)X + v(t)Y) U(t)$$
(1)

where

$$A := \begin{bmatrix} i & 0\\ 0 & -i \end{bmatrix},$$

$$X := \begin{bmatrix} 0 & -1\\ 1 & 0 \end{bmatrix},$$

$$Y := \begin{bmatrix} 0 & i\\ i & 0 \end{bmatrix}$$
(2)

and where c, u and v are functions of time describing the temporal variations of the external field. In our case we shall treat $t \mapsto u(t)$ and $t \mapsto v(t)$ as control functions whereas c is a constant (so that cA is a drift term in the system dynamics). Our goal will be to steer the system state from a given value U(0) at time t = 0 to a specified value $U(\tau)$ at time $\tau > 0$ in such a way that a cost functional of the form

$$\int_0^\tau \Phi(u(t), v(t)) \mathrm{d}t \tag{3}$$

(depending only on the controls, not on the state) becomes minimal. In applications one is mainly interested in the time-optimal case (in which $\Phi(u, v) \equiv 1$) either under the constraints $|u| \leq 1$ and $|v| \leq 1$ or under the more severe constraint $u^2 + v^2 \leq 1$. However, we shall also discuss the case $\Phi(u, v) = (1/2)(u^2 + v^2)$ (with no constraints on u and v), in which the optimal controls can be found rather easily. This case can then be compared to the time-optimal case, as follows: Determine (analytically, if possible) the optimal controls $t \mapsto u(t; \tau)$ and $t \mapsto v(t; \tau)$ in dependence on the given duration τ and find the minimal τ which is compatible with the constraints imposed in the time-optimal case.

2 Lie-theoretic Structure

Equation (1) is a control system evolving on the group SU(2) of all complex (2×2) -matrices U such that $U^*U = 1$ and det(U) = 1; equivalently,

$$\mathbf{SU}(2) = \left\{ \begin{bmatrix} a & -\overline{c} \\ c & \overline{a} \end{bmatrix} \mid a, c \in \mathbb{C}, |a|^2 + |c|^2 = 1 \right\}.$$
(4)

Note that the system (1) is right-invariant in the sense that if $t \mapsto U(t)$ is a trajectory of (1) then so is $t \mapsto U(t)B$ for any fixed $B \in SU(2)$. (This, by the way, ensures that we can always assume that U(0) = 1; otherwise we can replace U by $U(t)U(0)^{-1}$, which satisfies the same equation as U.) The Lie algebra su(2) of SU(2) consists of all traceless skewHermitian (2×2) -matrices; it is spanned by the elements A, X and Y in (2), and these satisfy the bracket relations

For later purposes, we give an explicit formula for the exponential function of su(2). Given a matrix

$$M = \begin{bmatrix} ic & -\overline{z} \\ z & -ic \end{bmatrix} \in \mathfrak{su}(2) \quad (c \in \mathbb{R}, z \in \mathbb{C}) \qquad (6)$$

we let

$$S := \begin{bmatrix} \overline{z} & \overline{z} \\ i(c-\Delta) & i(c+\Delta) \end{bmatrix}$$
(7)

where

$$\Delta := \sqrt{c^2 + |z|^2} \tag{8}$$

and observe that

$$S^{-1}MS = \begin{bmatrix} i\Delta & 0\\ 0 & -i\Delta \end{bmatrix} =: D \tag{9}$$

so that $M = SDS^{-1}$ and hence $\exp(tM) = S\exp(tD)S^{-1}$ for all $t \in \mathbb{R}$. Explicitly, the last equation reads

$$\exp(tM) = \exp\left(t\begin{bmatrix}ic & -\overline{z}\\z & -ic\end{bmatrix}\right)$$
$$= \cos(t\Delta)\begin{bmatrix}1 & 0\\0 & 1\end{bmatrix} + \frac{\sin(t\Delta)}{\Delta}\begin{bmatrix}ic & -\overline{z}\\z & -ic\end{bmatrix}$$
(10)
$$= \cos(t\sqrt{\det(M)})\mathbf{1} + \frac{\sin(t\sqrt{\det(M)})}{\sqrt{\det(M)}}M$$

where 1 denotes the identity matrix. This formula could also have been derived from the Hamilton-Cayley Theorem $M^2 - (trM)M + (\det M)\mathbf{1} = \mathbf{0}$ which, because of tr(M) = 0, becomes $M^2 = -\det(M)\mathbf{1}$. Consequently, we find that $M^{2k} = (-\det(M))^k \mathbf{1}$ and $M^{2k+1} = (-\det(M))^k M$ for all $k \in \mathbb{N}_0$; plugging these equations into the expansion $\exp(tM) = \sum_{r=0}^{\infty} t^r M^r / r!$, equation (10) follows.

We now exploit the Lie-theoretic structure inherent in the problem by invoking a version of Pontryagin's Maximum Principle which is tailor-made for right-invariant systems on Lie groups. This version states that, if u und v are optimally chosen, then there is an absolutely continuous function $p : [0, \tau] \rightarrow$ su(2) satisfying the adjoint equation

$$\dot{p}(t) = -p(t) \circ \operatorname{ad}(cA + u(t)X + v(t)Y) \quad (11)$$

and never becoming zero, which is such that u(t) and v(t) minimize the Hamiltonian

$$H = \chi \cdot \Phi(u, v) + c \cdot p(t) A + u \cdot p(t) X + v \cdot p(t) Y \quad (12)$$

(where $\chi \in \{0,1\}$) with respect to u and v almost everywhere; moreover, the Hamiltonian is constant along the optimal trajectory and control, the constant being zero if the final time τ is not fixed beforehand. (The abnormal case $\chi = 0$ will not be of significance in the problems at hand.) Applying (11) to A, X and Y, respectively, and using the bracket relations (5) we obtain the equations

$$\dot{p}(t)A = -p(t)(2u(t)Y - 2v(t)X), \dot{p}(t)X = -p(t)(-2cY + 2v(t)A), \dot{p}(t)Y = -p(t)(-2cX - 2u(t)A).$$
(13)

Letting a(t) := p(t)A, x(t) := p(t)X and y(t) := p(t)Y this reads

$$\begin{bmatrix} \dot{a} \\ \dot{x} \\ \dot{y} \end{bmatrix} = \begin{bmatrix} -2uy + 2vx \\ 2cy - 2va \\ -2cx + 2ua \end{bmatrix}$$

$$= 2\begin{bmatrix} 0 & v & -u \\ -v & 0 & c \\ u & -c & 0 \end{bmatrix} \begin{bmatrix} a \\ x \\ y \end{bmatrix}$$
(14)

which implies that $a(t)^2 + x(t)^2 + y(t)^2$ ist constant. Note that (14) holds irrespectively of the choice of the penalty function Φ . This choice, however, determines how the optimal controls u and v can be expressed in terms of the functions a, x and y, as will be discussed now.

3 Energy-Optimal Control

Let us choose $\Phi(u, v) := (1/2) \cdot (u^2 + v^2)$. We want to first rule out the abnormal case $\chi = 0$. Assume $\chi = 0$; then the absence of constraints on the controls u and v ensures that $x \equiv 0$ and $y \equiv 0$. Plugging this into (14) yields $\dot{a} = 0$, 0 = -2va and 0 = 2ua. Hence a is a constant; in fact a nonzero constant, because otherwise we would have $p \equiv 0$. But then $u \equiv 0$ and $v \equiv 0$, which yields a solution only if the uncontrolled system automatically reaches the desired state at time τ , a trivial case which can be discarded. Hence we may assume $\chi = 1$ so that the Hamiltonian (12) becomes

$$H = \frac{u^2 + v^2}{2} + c a(t) + u x(t) + v y(t). \quad (15)$$

Minimization of (15) with respect to u and v results in

$$\begin{array}{lll} u(t) &=& -x(t), \\ v(t) &=& -y(t). \end{array}$$
 (16)

Plugging this into (14) yields $\dot{a} = 0$ (so that a is a constant) and then $\dot{x} = 2(c+a)y$ and $\dot{y} = -2(c+a)x$, which implies that there are a constant r and a function φ such that $x(t) = r \cos(\varphi(t))$ and $y(t) = r \sin(\varphi(t))$ and $\dot{\varphi} = -2(c+a)$, i.e.,

$$u(t) = -r\cos(\varphi(t)),$$

$$v(t) = -r\sin(\varphi(t))$$
(17)

where

$$\varphi(t) = \varphi_0 - 2(c+a)t. \tag{18}$$

Hence the optimal trajectory satisfies $\dot{U}(t) = \Theta(t)U(t)$ where

$$\Theta(t) := cA + r\cos(\varphi(t))X + r\sin(\varphi(t))Y$$

= $c \begin{bmatrix} i & 0\\ 0 & -i \end{bmatrix} + r \begin{bmatrix} 0 & -e^{-i\varphi}\\ e^{i\varphi} & 0 \end{bmatrix};$ (19)

it remains to adjust the constants a, r and φ_0 in such a way that the desired change from $U(0) = \mathbf{1}$ to $U(\tau)$ is effected. We now use a trick to convert the equation $\dot{U} = \Theta U$ (which is a linear differential equation with time-varying coefficients) into a linear differential equation with constant coefficients by introducing the function $t \mapsto T(t) \in SU(2)$ defined by

$$T := \frac{1}{\sqrt{2}} \begin{bmatrix} e^{i\varphi/2} & -e^{-i\varphi/2} \\ e^{i\varphi/2} & e^{-i\varphi/2} \end{bmatrix}.$$
 (20)

We observe that both

$$T\begin{bmatrix}i & 0\\ 0 & -i\end{bmatrix}T^{-1} = \begin{bmatrix}0 & i\\ i & 0\end{bmatrix} = Y$$
(21)

and

$$T\begin{bmatrix} 0 & -e^{-i\varphi} \\ e^{i\varphi} & 0 \end{bmatrix} T^{-1} = \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix} = X \quad (22)$$

are constant in time, which is also true of

$$\dot{T}T^{-1} = \frac{\dot{\varphi}}{2} \begin{bmatrix} 0 & i \\ i & 0 \end{bmatrix} = -(c+a) \cdot Y.$$
 (23)

Thus the function

$$V(t) := T(t)U(t) \tag{24}$$

satisfies

$$\dot{V} = \dot{T}U + T\dot{U} = \dot{T}U + T\Theta U
= (\dot{T}T^{-1} + T\Theta T^{-1})TU
= (\dot{T}T^{-1} + T\Theta T^{-1})V
= (-(c+a)Y + cY + rX)V
= (rX - aY)V,$$
(25)

which has constant coefficients; in fact, letting

$$z := r - ia \tag{26}$$

this equation simply reads

$$\dot{V}(t) = A_z V(t)$$
 where $A_z := \begin{bmatrix} 0 & -\overline{z} \\ z & 0 \end{bmatrix}$ (27)

which can be explicitly solved, using U(0) = 1, to yield

$$V(t) = \exp(tA_z)V(0) = \frac{1}{\sqrt{2}}\exp(tA_z) \begin{bmatrix} e^{i\varphi_0/2} & -e^{-i\varphi_0/2} \\ e^{i\varphi_0/2} & e^{-i\varphi_0/2} \end{bmatrix}.$$
 (28)

Introducing the abbreviations

$$\begin{array}{ll} \alpha \ := \ \varphi_0/2 \quad \text{and} \\ \beta \ := \ \varphi(\tau)/2 \ = \ \alpha - (c+a)\tau \end{array} \tag{29}$$

and using the fact that $U(t) = T(t)^{-1}V(t) = T(t)^{\star}U(t)$, this yields

$$U(t) = \frac{1}{2} \begin{bmatrix} e^{-i\beta} & e^{-i\beta} \\ -e^{i\beta} & e^{i\beta} \end{bmatrix} \exp(tA_z) \begin{bmatrix} e^{i\alpha} & -e^{-i\alpha} \\ e^{i\alpha} & e^{-i\alpha} \end{bmatrix}.$$
(30)

Using (10) with c = 0 at the final time $t = \tau$, we find that

$$\exp(\tau A_z) = \begin{bmatrix} C & -S \\ S & C \end{bmatrix}$$
(31)

where

$$C := \cos(\tau |z|) \quad \text{and} \quad S := \frac{z}{|z|} \sin(\tau |z|); \quad (32)$$

a subsequent evaluation of (30) then yields

$$U(\tau) = \begin{bmatrix} e^{i(\alpha-\beta)}(C+i\Im S) & -e^{-i(\alpha+\beta)} \cdot \Re S \\ e^{i(\alpha+\beta)} \cdot \Re S & e^{i(\beta-\alpha)}(C-i\Im S) \end{bmatrix}.$$
(33)

Denoting by U_{ij} the entries of $U(\tau)$, we see from (33) that $e^{i(\beta-\alpha)}U_{11} = C + i \cdot \Im S$; thus if P is the polar angle of $U_{11} \in \mathbb{C}$ (so that $U_{11} = |U_{11}|e^{iP}$) we have

$$|U_{11}|e^{i(\beta-\alpha+P)} = C + i \cdot \Im S. \tag{34}$$

$$\begin{array}{lll}
\theta & := & -a\tau, \\
\theta_0 & := & c\tau - P, \\
w & := & \tau |z| = \tau \sqrt{r^2 + a^2}
\end{array}$$
(35)

(where θ_0 is a known constant whereas θ and w are unknowns because a and r are) we have $\theta - \theta_0 = P - (c+a)\tau = P + \beta - \alpha$; hence (34) takes the form

$$|U_{11}| \cdot \begin{bmatrix} \cos(\theta - \theta_0) \\ \sin(\theta - \theta_0) \end{bmatrix} = \begin{bmatrix} \cos(w) \\ \theta \cdot \sin(w)/w \end{bmatrix}.$$
 (36)

Taking norms on both sides of (34) we find that $|U_{11}|^2 = \cos(w)^2 + \theta^2 \sin(w)^2/w^2$ and hence that

$$\theta = \frac{\varepsilon w \sqrt{|U_{11}|^2 - \cos^2 w}}{\sin w} \tag{37}$$

where $\varepsilon \in \{\pm 1\}$. Furthermore, (36) implies that $\tan(\theta - \theta_0) = \theta \tan(w)/w$ and hence that

$$\tan\left[\frac{\varepsilon w \sqrt{|U_{11}|^2 - \cos^2 w}}{\sin w} - \theta_0\right]$$

$$= \frac{\varepsilon \sqrt{|U_{11}|^2 - \cos^2 w}}{\cos w}.$$
(38)

This equation has more than one solution, but since the control effort is given by

$$\int_{0}^{\tau} \Phi(u, v) dt = \int_{0}^{\tau} \frac{u^{2} + v^{2}}{2} dt = \frac{r^{2}\tau}{2}$$
$$= \frac{\tau}{2} \left(\frac{w^{2}}{\tau^{2}} - a^{2}\right) = \frac{w^{2} - \tau^{2}a^{2}}{2\tau}$$
$$= \frac{w^{2} - \theta^{2}}{2\tau} = \frac{1 - |U_{11}|^{2}}{2\tau} \frac{w^{2}}{\sin^{2} w},$$
(39)

we are looking, amongst all possible solutions, for the one for which $|w/\sin(w)|$ is minimal. Once (38) has been solved for w, we plug the result into (37) to obtain θ , then let $a := -\theta/\tau$ and $r := \sqrt{(w/\tau)^2 - a^2}$ according to (35); finally, φ_0 can be determined from

$$-\frac{U_{21}}{U_{12}} = e^{2i(\alpha+\beta)} = e^{2i(\varphi_0 - c\tau - a\tau)}.$$
 (40)

Once a, r and φ_0 are found, the optimal controls are given by

$$u(t) = -x(t) = -r \cdot \cos(\varphi_0 - 2(c+a)t),$$

$$v(t) = -y(t) = -r \cdot \sin(\varphi_0 - 2(c+a)t).$$
(41)

The special case $U_{11} = 0$ is particularly simple. In this case necessarily $|U_{21}| = 1$, say $U_{21} = e^{i\sigma}$. Equation (36) implies that $\cos(w) = 0$ and $\theta = 0$, hence a = 0 and $w = \tau r$; the equation $\cos(w) = 0$ thus yields $\tau r = (\pi/2) + k\pi$ with $k \in \mathbb{Z}$. Finally, equation (40) becomes $e^{2i\sigma} = e^{2i(\varphi_0 - c\tau)}$ so that $\varphi_0 \in \sigma + c\tau + \pi \cdot \mathbb{Z}$. (Note that φ_0 enters the control law only modulo 2π .) The value k has to be chosen to make |r|as small as possible; since one of the choices k = 0and k = -1 always gives a solution, we find that

$$u(t) = \varepsilon \cdot (\pi/(2\tau)) \cdot \cos(\sigma + c\tau - 2ct),$$

$$v(t) = \varepsilon \cdot (\pi/(2\tau)) \cdot \sin(\sigma + c\tau - 2ct),$$
(42)

where $\varepsilon \in \{\pm 1\}$ in (42) must be chosen in such a way that the resulting trajectory $t \mapsto U(t)$ leads to the desired state $U(\tau)$.

To see a numerical example, let us choose c:=1, $\tau:=\pi/2$ and

$$U(\tau) := \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & -1\\ 1 & 1 \end{bmatrix}$$

Plotting the difference of the left-hand side and the right-hand side of (38) yields the following diagram in which the thick solid lines and the thick dashed lines correspond to the cases $\varepsilon = 1$ and $\varepsilon = -1$, respectively, whereas the thin dashed line is the graph of the function $t \mapsto |w/\sin(w)|$.



Figure 1: Determination of the parameter w.

The solution of (38) yielding the minimal value of $|w/\sin(w)|$ is w = 2.21928. Each of the two possibilities $\varepsilon = \pm 1$ yields θ , a und r uniquely and then $\varphi_0 = (c+a)\tau + k\pi$ with a single ambiguity. Checking the four possibilities shows that the sought solution is given by $\varepsilon = -1$, r = 1.25348, a = 0.651835 and $\varphi_0 = 2.5947$. The four solutions obtained for the various choices all yield final states $U(\tau) \in SU(2)$ with $|U_{ij}| = 1/\sqrt{2}$ for $1 \le i, j \le 2$, but with the different sign combinations

$$\begin{bmatrix} - & - \\ + & - \end{bmatrix}, \begin{bmatrix} + & - \\ + & + \end{bmatrix}, \begin{bmatrix} - & + \\ - & - \end{bmatrix}, \begin{bmatrix} + & + \\ - & + \end{bmatrix}$$

4 Time-optimal Control: First Case

We now consider the question of time-optimal control (i.e., with the cost function $\Phi(u, v) = 1$) under the constraint $u^2 + v^2 \leq 1$. In this case minimization of (12) yields

$$u = \frac{-x}{\sqrt{x^2 + y^2}}, \quad v = \frac{-y}{\sqrt{x^2 + y^2}}.$$
 (43)

Plugging this into (14) results in $\dot{a} = 0$ (so that a is constant) and the system

$$\dot{x} = \frac{2cy + 2ay}{\sqrt{x^2 + y^2}}$$

$$\dot{y} = -2cx - 2ax/\sqrt{x^2 + y^2}$$
(44)

from which we conclude that $x\dot{x} + y\dot{y} = 0$, i.e., that $x^2 + y^2$ is constant. Hence there exist a constant r and a function φ such that $x(t) = r\cos(\varphi(t))$ and $y(t) = r\sin(\varphi(t))$ which, when plugged back into (44), yields $\dot{\varphi} = -2(c + (a/r))$ and hence that

$$\varphi(t) = \varphi_0 - 2\left(c + \frac{a}{r}\right)t.$$
 (45)

This is a solution of the same form as the one found in the energy-optimal case; we simply have to replace a by a/r. (This shows that the time-optimal control under the given constraint can be obtained by finding, for a given $\tau > 0$, the solution for the energy-optimal problem and then selecting the smallest τ for which the solution thus found is compatible with the constraint $u^2 + v^2 \le 1$.) However, since a and r enter the control law only via the quotient a/r, we may assume r = 1 without loss of generality; thus

$$u(t) = -\cos(\varphi(t)),$$

$$v(t) = -\sin(\varphi(t))$$
(46)

where

$$\varphi(t) = \varphi_0 - 2(c+a)t. \qquad (47)$$

The situation differs from the energy-optimal case in that τ is now not a given constant, but an unknown parameter to be determined. In order to identify the constants a, φ_0 and τ which yield the optimal control law, we can proceed as in the previous section up to equation (34). Using r = 1, this equation now takes the form

$$|U_{11}| \begin{bmatrix} \cos(P - (c+a)\tau) \\ \sin(P - (c+a)\tau) \end{bmatrix}$$

$$= \begin{bmatrix} \cos(\tau\sqrt{1+a^2}) \\ -a\sin(\tau\sqrt{1+a^2})/\sqrt{1+a^2} \end{bmatrix}$$
(48)

which yields

$$\tan(P - (c+a)\tau) = \frac{-a}{\sqrt{1+a^2}} \tan(\tau\sqrt{1+a^2}) \quad (49)$$

and, after taking norms, also shows that $|U_{11}|^2$ equals $\cos^2(\tau\sqrt{1+a^2}) + a^2\sin^2(\tau\sqrt{1+a^2})/(1+a^2)$ so that the equation

$$|U_{11}|^2 = \frac{\cos^2(\tau\sqrt{1+a^2}) + a^2}{1+a^2}$$
(50)

holds. This last equation implies that

$$\tau\sqrt{1+a^2} = \arccos\left(\pm\sqrt{(1+a^2)|U_{11}|^2 - a^2}\right) + k\pi$$
(51)

for some $k \in \mathbb{Z}$. Solving for τ and plugging the result into (49) yields an equation for a, and then φ_0 can be obtained from (40) above (which is still valid because, since r = 1, the function φ has the same form as in the previous discussion). Amongst all possible solutions (a, τ, φ_0) we must identify the one for which τ is minimal. Again, the case $U_{11} = 0$ is particularly simple. In this case (50) implies that a = 0 and $\tau = (\pi/2) + k\pi$ where $k \in \mathbb{N}_0$. Writing $U_{21} = e^{i\sigma}$, we find again that $\varphi_0 \in \sigma + c\tau + \pi \cdot \mathbb{Z}$.

5 Time-optimal Control: Second Case

We consider again the case $\Phi(u, v) = 1$ (i.e., the case of time-optimal control), but this time with the individual control constraints $|u| \le 1$ and $|v| \le 1$ instead of the more severe overall constraint $u^2 + v^2 \le 1$. In this case minimization of (12) yields

$$u(t) = -\operatorname{sign}(x(t)) \text{ and} v(t) = -\operatorname{sign}(y(t))$$
(52)

unless there is an interval on which $x \equiv 0$ or $y \equiv 0$ (in which case u or v could not be determined on this interval from minimizing (12)). Let us show that this is only possible if both $u \equiv 0$ and $v \equiv 0$, so

that the only possible singular arcs are drift arcs (also called coast arcs) during which no control whatsoever is applied. (It will become clear from the subsequent discussion that generically those arcs do not occur and can be ignored as far as practical implementation of an optimal control scheme is concerned.) Assume that $x \equiv 0$ on some time interval. Then, according to (14), on this time interval the following equations hold:

$$\begin{bmatrix} \dot{a} \\ \dot{y} \end{bmatrix} = 2u \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} a \\ y \end{bmatrix}, \quad va = cy. \quad (53)$$

Denoting by U an antiderivative of u and letting $C(t) := \cos(2U(t))$ and $S(t) := \sin(2U(t))$, we find from the first equation in (53) that

$$\begin{bmatrix} a(t) \\ y(t) \end{bmatrix} = \begin{bmatrix} C(t) & -S(t) \\ S(t) & C(t) \end{bmatrix} \begin{bmatrix} a_0 \\ y_0 \end{bmatrix}.$$
(54)

Apart from the trivial cases $a_0 = y_0 = 0$ and U(t) = const, this implies (because of the second equation in (53)) that

$$v(t) = c \cdot \frac{y(t)}{a(t)} = c \cdot \frac{a_0 S(t) + y_0 C(t)}{a_0 C(t) - y_0 S(t)}$$
(55)

is not constant on any part of the time interval considered unless $y \equiv 0$ on this interval. But then $x \equiv 0$ and $y \equiv 0$ on this interval, which (as we saw in the discussion preceding (15)) implies $u \equiv 0$ and $v \equiv 0$. Let us discuss the two trivial cases mentioned before. If $a_0 = y_0 = 0$ then (54) implies $y \equiv 0$, and we again obtain x = y = 0 and hence u = v = 0. If U is constant, then $u \equiv 0$, hence a and y are also constant. The Hamiltonian is then given by H = ca + vy. The fact that the Hamiltonian is zero along an optimal trajectory, together with the second equation in (53), gives rise to the equation

$$\begin{bmatrix} v & -c \\ c & v \end{bmatrix} \begin{bmatrix} a \\ y \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$
(56)

and hence that a = y = 0 and consequently u = v = 0 again. This confirms our claim that the only possible singular arcs are coast arcs during which no controls are applied.

Ignoring coast arcs for the time being, the time interval $[0, \tau]$ splits into intervals on which both u and v are constant with values in $\{\pm 1\}$. On each such interval equation (14) becomes

$$\begin{bmatrix} \dot{a} \\ \dot{x} \\ \dot{y} \end{bmatrix} = 2 \begin{bmatrix} 0 & v & -u \\ -v & 0 & c \\ u & -c & 0 \end{bmatrix} \begin{bmatrix} a \\ x \\ y \end{bmatrix}$$
(57)

which is an equation with constant coefficients which can be explicitly integrated as

$$\begin{bmatrix} a(t)\\ x(t)\\ y(t) \end{bmatrix} = \exp\left(2(t-s)\begin{bmatrix} 0 & v & -u\\ -v & 0 & c\\ u & -c & 0 \end{bmatrix}\right) \begin{bmatrix} a(s)\\ x(s)\\ y(s) \end{bmatrix}$$
(58)

where the exponential can be computed using the Rodrigues formula which states that for any skewsymmetric matrix

$$L(\omega) = \begin{bmatrix} 0 & -\omega_3 & \omega_2 \\ \omega_3 & 0 & -\omega_1 \\ -\omega_2 & \omega_1 & 0 \end{bmatrix}$$
(59)

where $\omega = (\omega_1, \omega_2, \omega_3)^T \in \mathbb{R}^3$ the exponential $\exp(L(\omega))$ is given by

$$(\cos \|\omega\|)\mathbf{1} + \frac{1 - \cos \|\omega\|}{\|\omega\|^2} \omega \otimes \omega + \frac{\sin \|\omega\|}{\|\omega\|} L(\omega).$$
(60)

Thus if [s, t] is a time interval during which u and v are constant (with values in $\{\pm 1\}$), we have $\omega = -2(c, u, v)^T$; hence (58) holds with the exponential given by

$$\cos(2(t-s)\sqrt{c^{2}+2}) \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} + \frac{1-\cos(2(t-s)\sqrt{c^{2}+2})}{c^{2}+2} \begin{bmatrix} c^{2} & uc & vc \\ uc & 1 & uv \\ vc & uv & 1 \end{bmatrix} \quad (61) + \frac{\sin(2(t-s)\sqrt{c^{2}+2})}{\sqrt{c^{2}+2}} \begin{bmatrix} 0 & v & -u \\ -v & 0 & c \\ u & -c & 0 \end{bmatrix}.$$

Let us note that the motion of the vector $(a, x, y)^T$ during the time interval [s, t] is a rotation with constant angular velocity $\sqrt{c^2 + 2}$ about the axes pointing in the direction of $(c, u, v)^T$; hence

$$2(t-s)\sqrt{c^2+2} = 2\Phi_{t,s}$$
 (62)

where $\Phi_{t,s}$ is the angle swept out by this vector.

Depending on the four possibilities $(u, v) = (\pm 1, \pm 1)$, there are four possible axes of rotation; the larger |c|, the closer these axes are towards the *a*-axis in the adjoint space. The diagram shows a view from top (i.e., from the positive *a*-axis) onto the *xy*-plane. The adjoint variables evolve on a sphere



Figure 2: Evolution of adjoint variables.

 $a^2 + x^2 + y^2 = R^2$; around each of the four axes there is a circle which touches both the plane x = 0and the plane y = 0. If (a_0, x_0, y_0) lies in the interior of any such circle, no switching can occur, because then the trajectory $t \mapsto (a(t), x(t), y(t))$ can never leave the quadrant in which it starts. The exterior of the union of these four circles is composed of two regions; region I containing the point (R, 0, 0), region II containing the point (0, 0, R). If c < 0 the positively oriented rotation axes "stick out" of the diagram, so that the motion along the circles is in the mathematically positive sense. Thus if (a_0, x_0, y_0) is in region I, we follow the switching pattern

u	-1	-1	1	1
v	-1	1	1	-1

(traversing the four quadrants of the xy-plane in clockwise fashion), whereas if (a_0, x_0, y_0) is in region II, we follow the switching pattern



(traversing the four quadrants in counterclockwise fashion). This motion in the adjoint space needs to be strictly distinguished from the associated motion in the state space SU(2) which is determined from the switching pattern by the fact that on each time interval

on which u and v are constant the state equation (1) becomes

$$\dot{U}(t) = \begin{bmatrix} ci & -u+iv\\ u+iv & -ci \end{bmatrix} U(t)$$
(63)

which is also an equation with constant coefficients and hence can be explicitly integrated via

$$U(t) = \exp\left((t-s) \begin{bmatrix} ci & -u+iv\\ u+iv & -ci \end{bmatrix}\right) U(s) \quad (64)$$

where the exponential can be evaluated using (10). The remaining step is to determine the control synthesis (yielding for each desired target state the times at which switchings in the optimal control functions occur), which in particular requires deriving an upper bound for the number of possible switchings. This is not a trivial task and will be described in a subsequent paper. Possible approaches are the symplectic techniques developed by Agrachev et al. (see [1], [2]) or Sussmann's envelope method (see [5], [6]), but in our problem a simpler approach is possible because reduction to a two-dimensional problem is possible, as follows. Consider the Hopf map, i.e., the mapping $\Phi : SU(2) \rightarrow S^2$ given by

$$\begin{bmatrix} B & -\overline{C} \\ C & \overline{B} \end{bmatrix} \mapsto \begin{bmatrix} \xi_1 \\ \xi_2 \\ \xi_3 \end{bmatrix} := \begin{bmatrix} -2\Im(\overline{B}C) \\ 2\Re(\overline{B}C) \\ |B|^2 - |C|^2 \end{bmatrix}. \quad (65)$$

(This is really a mapping into \mathbb{S}^2 because $\xi_1^2 + \xi_2^2 + \xi_3^2 = 4|\overline{B}C|^2 + (|B|^2 - |C|^2)^2 = (|B|^2 + |C|^2)^2 = 1.)$ Note that the system dynamics (1) can be rewritten as

$$\dot{B} = ciB - uC + viC
\dot{C} = -ciC + uB + viB$$
(66)

which, when plugged into (65), yields

$$\begin{bmatrix} \dot{\xi}_3\\ \dot{\xi}_1\\ \dot{\xi}_2 \end{bmatrix} = 2 \begin{bmatrix} 0 & v & -u\\ -v & 0 & c\\ u & -c & 0 \end{bmatrix} \begin{bmatrix} \xi_3\\ \xi_1\\ \xi_2 \end{bmatrix}, \quad (67)$$

an equation which coincides with the adjoint equation (14). Since (67) is a control system evolving on a two-dimensional manifold, the techniques described in [4] are applicable to determine an upper bound for the number of switchings for the optimal controls in (67). Now if $t \mapsto u(t)$ and $t \mapsto v(t)$ are controls which optimally steer system (67) from ξ_0 to ξ_1 in time τ and if $t \mapsto g(t)$ is any trajectory in SU(2) resulting from these controls, then this latter trajectory

is automatically an optimal trajectory joining the initial state g(0) to the final state $g(\tau)$. This simple observation can then be used to derive an upper bound for the number of control switchings for system (1) in terms of those for system (67); cf. [3] in which this technique was applied to a system without drift.

A second approach is based on the application of second-order conditions for optimality (in addition to the necessary first-order condition provided by the Maximum Principle) in a way introduced by Agrachev and Gamkrelidze; see [1]. Consider a control system on a Lie group G which has the form

$$\dot{g}(t) = U(t)g(t) \tag{68}$$

where $U(t) = \sum_i u_i(t)E_i$ with control functions u_i (subject to pointwise bounds) and Lie algebra generators E_i . (The system (1) we are interested in is of this form. Note that the letter U is now used with a different meaning than before.) We start with a reference control $t \mapsto U^*(t)$ (assumed to be time-optimal, with minimal time T) and the resulting reference trajectory $t \mapsto g^*(t)$ satisfying

$$\dot{g}^{\star}(t) = U^{\star}(t)g^{\star}(t).$$
 (69)

We now consider a reparametrization $t \mapsto \theta(t)$ of time which is small in the sense that $\dot{\theta}(t)$ stays close to 1, say $\dot{\theta}(t) = 1 + w(t)$ where w is small. We introduce the modified control system

$$\dot{g}(t) = (1+w(t))U^{\star}(t)g(t)
\dot{\theta}(t) = 1+w(t)$$
(70)

with w as a single control variable; we claim that $t \mapsto g^*(t)$ is time-optimal for the problem of steering (70) from the initial state $(g_0, 0)$ to the target state (g_1, T) (where T is the minimum time required to steer (68) from g_0 to g_1). To show this, assume that there is a control steering the modified system to a state (g_1, S) with S < T. Define $\gamma(\tau) := g(\theta^{-1}(\tau))$ for $0 \le t \le \theta(S)$. Taking derivatives on both sides of the equation $g(t) = \gamma(\theta(t))$, we find that

$$(1+w)U^{*}g = \dot{g} = (\dot{\gamma} \circ \theta)\dot{\theta} = (1+w)(\dot{\gamma} \circ \theta).$$
(71)

Dividing by 1 + w and writing $\tau = \theta(t)$, this becomes

$$U^{\star}(\theta^{-1}(\tau))\gamma(\tau) = \dot{\gamma}(\tau) \tag{72}$$

which shows that γ is a trajectory of the original system (68). (Note that $U^* \circ \theta^{-1}$ is an admissible control since U^* is.) Moreover, $\gamma(0) = g(0) = g_0$

and $\gamma(\theta(S)) = g(S) = g_1$. Since θ strictly increases, we have $\theta(S) < \theta(T) = T$; thus the control $\hat{U}(t) := U^*(\theta^{-1}(t))$ steers the original system from g_0 to g_1 in a time smaller than T, contradicting our hypothesis of T being the optimal time. Now let w be a sufficiently small control steering the system (70) from (g(0), 0) to (g(T), T), let (g_w, θ_w) be the resulting trajectory of (70) and let

$$x_w(t) := g^*(t)^{-1}g_w(t)$$
 (73)

be the deviation between g_w and g^* . Then, using the first equation in (70), we find that

$$(1+w)U^{*}g^{*}x_{w} = (1+w)U^{*}g_{w} = \dot{g}_{w} = (d/dt)(g^{*}x_{w}) = \dot{g}^{*}x_{w} + g^{*}\dot{x}_{w} = U^{*}g^{*}x_{w} + g^{*}\dot{x}_{w}.$$
(74)

Subtracting $U^*g^*x_w$ from both sides of (74), we find that $wU^*g^*x_w = g^*\dot{x}_w$; i.e., letting

$$H(t) := g^{\star}(t)^{-1} U^{\star}(t) g^{\star}(t), \qquad (75)$$

we see that $t \mapsto x_w(t)$ is a solution of the differential equation

$$\dot{x}(t) = w(t)H(t)x(t)$$
. (76)

Consequently,

$$x(T) = x(0) + \int_0^T \dot{x}(\tau_1) \, \mathrm{d}\tau_1$$

= $x(0) + \int_0^T w(\tau_1) H(\tau_1) x(\tau_1) \, \mathrm{d}\tau_1$. (77)

Plugging the first equation of (77) (with T replaced by τ_1) into the second we find that x(T) equals

$$x(0) + \int_{0}^{T} w(\tau_1) H(\tau_1) \left[x(0) + \int_{0}^{\tau_1} \dot{x}(\tau_2) \, \mathrm{d}\tau_2 \right] \mathrm{d}\tau_1 \quad (78)$$

so that

$$x(T) = x(0) + \int_0^T w(\tau_1) H(\tau_1) x(0) \, \mathrm{d}\tau_1 + \int_0^T \int_0^{\tau_1} w(\tau_1) H(\tau_1) w(\tau_2) H(\tau_2) x(\tau_2) \, \mathrm{d}\tau_2 \, \mathrm{d}\tau_2 \,.$$
(79)

Continuing in this way, we see that the endpoint-map

$$\mathfrak{E}[w] := x_w(T) \tag{80}$$

which maps each admissible control w to the point of the resulting trajectory of (70) at time T, is given by the Volterra series

$$\mathfrak{E} = \mathbf{1} + \sum_{k=1}^{\infty} \int_{\Delta_k} \prod_{i=1}^k w(\tau_i) H(\tau_i) \, \mathrm{d}(\tau_1, \dots, \tau_k) \quad (81)$$

where $\Delta_k := \{(\tau_1, \ldots, \tau_k) \in \mathbb{R}^k \mid 0 \le \tau_1 \le \cdots \le \tau_k \le T\}$. Now the control w = 0 is a critical point of the endpoint map so that $\mathfrak{E}'[0]$ has a nontrivial kernel. Since

$$\mathfrak{E}'[0]w = \int_0^T w(\tau)H(\tau) \,\mathrm{d}\tau \,, \qquad (82)$$

this implies that there is a nonzero element $p \in L(G)^*$ (where L(G) denotes the Lie algebra of G) such that

$$0 = p\left[\int_{0}^{T} w(t)H(t) dt\right]$$

=
$$\int_{0}^{T} w(t) p(H(t)) dt$$
(83)

for all w such that $\int_0^T w(t) dt = 0$. This clearly implies that p(H(t)) is constant for $0 \le t \le T$. (To wit: using the constant function 1, the above condition can be written as $p \circ H \in (1^{\perp})^{\perp} = \mathbb{R} \cdot 1$ with respect to the inner product $\langle f, g \rangle = \int_0^T fg$.) Now let

$$I_{1} := \iint_{0 \le \tau_{1} \le \tau_{2} \le T} w(\tau_{1})w(\tau_{2})H(\tau_{1})H(\tau_{2}) d(\tau_{1},\tau_{2}),$$

$$I_{2} := \iint_{0 \le \tau_{1} \le \tau_{2} \le T} w(\tau_{1})w(\tau_{2})H(\tau_{2})H(\tau_{1}) d(\tau_{1},\tau_{2}).$$
(84)

Clearly

$$I_{2} = \iint_{0 \le \tau_{2} \le \tau_{1} \le T} w(\tau_{2}) w(\tau_{1}) H(\tau_{1}) H(\tau_{2}) d(\tau_{1}, \tau_{2}) \quad (85)$$

so that

$$I_{1}+I_{2} = \iint_{\substack{0 \le \tau_{1}, \tau_{2} \le T \\ T}} w(\tau_{1})w(\tau_{2})H(\tau_{1})H(\tau_{2}) d(\tau_{1}, \tau_{2}) \\ = \left(\int_{0}^{T} w(\tau_{1})H(\tau_{1}) d\tau_{1}\right) \left(\int_{0}^{T} w(\tau_{2})H(\tau_{2}) d\tau_{2}\right) (86) \\ = \left(\int_{0}^{T} w(\tau)H(\tau) d\tau\right)^{2}.$$

Now if w is in the kernel of $\mathfrak{E}'[0]$, this last integral vanishes, and we have $I_1 + I_2 = 0$ so that $I_2 = -I_1$. But then $I_1 - I_2 = 2I_1$, so that I_1 (i.e., the second term in the above Volterra series) is given by $(I_1 - I_2)/2$. Thus (since $H_1H_2 - H_2H_1 = [H_1, H_2]$) we find that

$$I_{1} = \frac{1}{2} \iint_{0 \le \tau_{1} \le \tau_{2} \le T} w(\tau_{1}) w(\tau_{2}) \left[H(\tau_{1}), H(\tau_{2}) \right] \mathsf{d}(\tau_{1}, \tau_{2})$$
(87)

which is an element of the Lie algebra to which p can be applied. Since $w \mapsto p(x_w(T))$ takes an extremum at w = 0, this last expression must be a semidefinite quadratic form of w.

We now specialize to the case that U^* is a bangbang control and hence piecewise constant. Then H(t) is constant between two switching times t_i and t_{i+1} ; in fact, for all $t \in [t_i, t_{i+1})$ we have $U^*(t) = U^*(t_i)$, hence

$$g^{\star}(t) = \exp((t - t_i)U^{\star}(t_i))g(t_i)$$
 (88)

and consequently

$$H(t) = g^{\star}(t)^{-1}U^{\star}(t)g^{\star}(t) = g(t_i)^{-1}U^{\star}(t_i)g(t_i) = H(t_i).$$
(89)



Figure 3: Decomposition of integration domain.

Letting

$$y_i := \int_{t_i}^{t_{i+1}} w(\tau) \,\mathrm{d}\tau \,,$$
 (90)

we find that

$$\int_{0}^{T} \int_{0}^{t} w(t)w(\tau)p([H(t), H(\tau)]) d\tau dt$$

$$= \sum_{i \leq j} \int_{t_{i}}^{t_{i+1}} \int_{t_{j}}^{t_{j+1}} w(t)w(\tau)p([H(t_{j}), H(t_{i})]) d\tau dt$$

$$= \sum_{i < j} y_{i}y_{j} p([H(t_{j}), H(t_{i})]).$$
(91)

Thus one way to show that a bang-bang control ceases to be optimal is to prove that the quadratic form given by (91) is no longer semidefinite if another switching time is added. The calculations to do this for the problem at hand are elaborate and will be presented elsewhere.

6 Appendix

For those readers not acquainted with a coordinatefree treatment of control systems on manifolds we want to give a quick derivation of the version of Pontryagin's Principle used in this paper; this requires a differential-geometric interpretation of the Hamiltonian equations. Assume that a control system on a manifold is given and that a fixed control is chosen. The resulting trajectory is then the solution of an initial value problem

$$\dot{x}(t) = f(x(t), t), \quad x(s) = p.$$
 (92)

Let $\varphi_{ts}(p) = x(t; p, s)$ be the associated flow on M (so that $\varphi_{ts}(p)$ is the state at time t for the trajetory which at time s is in state p). This flow induces the tangent flow

$$\Phi_{ts}(p,v) := (\varphi_{ts}(p), \varphi'_{ts}(p)v)$$
(93)

on TM and, by dualization, the cotangent flow

$$\Psi_{ts}(p,\lambda) := (\varphi_{ts}(p), \lambda \circ \varphi'_{ts}(p)^{-1}) \qquad (94)$$

on T^*M . These two flows are such that $\lambda_t(v_t)$ is constant because

$$\lambda_t(v_t) = \left(\lambda_s \circ \varphi_{ts}'(p)^{-1}\right) \left(\varphi_{ts}'(p)v_s\right) = \lambda_s(v_s); \ (95)$$

in fact, the condition that $\lambda_t(v_t)$ is constant characterizes the cotangent flow. Now let us fix the initial time s. Then the variational equations for $\varphi_{ts}(p) = x(t;p)$ are given by

$$\frac{\mathrm{d}}{\mathrm{d}t}\varphi_{ts}'(p) = \frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial}{\partial p}x(t;p) = \frac{\partial}{\partial p}\frac{\mathrm{d}}{\mathrm{d}t}x(t;p)$$

$$= \frac{\partial}{\partial p}\dot{x}(t;p) = \frac{\partial}{\partial p}f(x(t;p),t)$$

$$= \frac{\partial f}{\partial x}(x(t;p),t) \cdot \frac{\partial x(t;p)}{\partial p}$$

$$= \frac{\partial f}{\partial x}(\varphi_{ts}(p),t) \cdot \varphi_{ts}'(p).$$
(96)

Since $t \mapsto \lambda(t)(\varphi'_{ts}(p)v)$ is constant we find that

$$0 = \dot{\lambda}(t) \left(\varphi_{ts}'(p)v\right) + \lambda(t) \left(\frac{\mathrm{d}}{\mathrm{d}t}\varphi_{ts}'(p)v\right)$$
$$= \dot{\lambda}(t) \left(\varphi_{ts}'(p)v\right) + \lambda(t) \left(\frac{\partial f}{\partial x}(\varphi_{ts}(p), t) \cdot \varphi_{ts}'(p)v\right)$$
$$= \dot{\lambda}(t) \left(\varphi_{ts}'(p)v\right) + \frac{\partial H}{\partial x} \left(\varphi_{ts}(p), t, \lambda(t)\right) \left(\varphi_{ts}'(p)v\right)$$
(97)

because $H(x,t,\lambda) = \lambda(f(x,t))$ satisfies

$$\frac{\partial H}{\partial x}(x,t,\lambda) \bullet = \lambda \left(\frac{\partial f}{\partial x}(x,t) \bullet\right).$$
(98)

This shows that (x_t, λ_t) is a solution of the Hamiltonian equations if and only if (x_t, λ_t) is a cotangent flow. The solution yielding the maximum condition is obtained by choosing λ_T at the final time such that the kernel of λ_T is a supporting hyperplane of the reachable set at time T. In an optimal control problem $\dot{x}(t) = f(x(t), u(t), t)$ with a cost functional $\int_{t_0}^T \varphi(x(t), u(t), t) dt$ this observation is applied to the augmented system

in which

$$c(t) := \int_{t_0}^t \varphi(x(\tau), u(\tau), \tau) \,\mathrm{d}\tau \tag{100}$$

is the running cost. For a system of the special form

$$\dot{g}(t) = U(t)g(t), \quad g(s) = g_0$$
 (101)

on a Lie group G the above derivation can be simplified. If we write the associated flow in the form

$$\varphi_{ts}(g_0) = g(t; g_0) \tag{102}$$

the variational equations become

$$\frac{\mathrm{d}}{\mathrm{d}t}\varphi_{ts}'(g_0) = \frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial}{\partial g_0}g(t;g_0) = \frac{\partial}{\partial g_0}\frac{\mathrm{d}}{\mathrm{d}t}g(t;g_0)$$

$$= \frac{\partial}{\partial g_0}\dot{g}(t;g_0) = \frac{\partial}{\partial g_0}U(t)g(t;g_0)$$

$$= U(t)\frac{\partial}{\partial g_0}g(t;g_0) = U(t)\varphi_{ts}'(g_0)$$
(103)

Defining $p(t) \in L(G)^*$ by

$$p(t)(Y) := \lambda(t)(Yg(t)) \tag{104}$$

for all elements $Y \in L(G)$ in the Lie algebra of G and introducing, for any fixed $X \in L(G)$, the function

$$\xi(t) := \varphi'_{ts}(g_0) X g(t)^{-1}, \qquad (105)$$

we see that

$$t \mapsto \lambda(t) \left(\varphi_{ts}'(g_0) X \right) = p(t) \left(\xi(t) \right)$$
 (106)

is constant. Now the derivative $\dot{\xi}(t)$ is given by

$$\left(\frac{\mathrm{d}}{\mathrm{d}t}\varphi_{ts}'(g_0)\right) Xg(t)^{-1} + \varphi_{ts}'(g_0) X\left(\frac{\mathrm{d}}{\mathrm{d}t}g(t)^{-1}\right)$$
(107)

which, since

$$\frac{\mathrm{d}}{\mathrm{d}t}\varphi_{ts}'(g_0) = U(t)\xi(t) \tag{108}$$

and

$$\frac{\mathrm{d}}{\mathrm{d}t}g(t)^{-1} = -g(t)^{-1}\dot{g}(t)g(t)^{-1}, \qquad (109)$$

means that

$$\dot{\xi}(t) = U(t)\xi(t) - \xi(t)U(t) = [U(t),\xi(t)]$$
. (110)

Since $t \mapsto p(t)(\xi(t))$ is constant, this implies that $0 = \dot{p}(\xi) + p(\dot{\xi}) = \dot{p}(\xi) + p([U,\xi])$ for all ξ of the above form and thus $0 = \dot{p} + p \circ ad(U)$, i.e.,

$$\dot{p}(t) = -p(t) \circ \mathrm{ad}(U(t)).$$
 (111)

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