Unitary operations acting on a quantum system must be robust against systematic errors in control parameters for reliable quantum computing. Composite pulse technique in nuclear magnetic resonance realizes such a robust operation by employing a sequence of possibly poor-quality pulses. In this study, we demonstrate that two kinds of composite pulses—one compensates for a pulse length error in a one-qubit system and the other compensates for a $J$-coupling error in a two-qubit system—have a vanishing dynamical phase and thereby can be seen as geometric quantum gates, which implement unitary gates by the holonomy associated with dynamics of cyclic vectors defined in the text.

**Keywords:** nuclear magnetic resonance; composite pulses; geometric phases; geometric quantum gates; quantum control

### 1. Introduction

Nuclear magnetic resonance (NMR) has developed many techniques to control physical systems and maintain their coherence [1,2]. A composite pulse is one such technique, in which a sequence of pulses is employed to cancel out a systematic error inherent in the pulses [3]. A systematic error is an unwanted imperfection in control parameters, such as poor calibration, and should not be confused with a random noise. The composite $\pi$-pulse of Levitt & Freeman [4], developed with intuitive but convincing account of its robustness, opened up a new field of research. Now we have hundreds of composite pulses [5,6] and dozens of methods to design them, such as iterative expansion [7], gradient ascent pulse engineering (GRAPE) [8,9] and concatenation [10].

Recently, quantum information processing (QIP) [12–15] has had an influence over the composite pulse design. Very accurate control of a quantum system is required for a successful quantum error correction, as shown by Gaitan [14], for example. Any quantum algorithm can be simulated by quantum circuits composed of one-qubit unitary operations and the controlled-NOT (CNOT) operations. As a result, robustness is required for arbitrary one-qubit operations

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and CNOT operation. In contrast, operations with limited angles and phases have been required in conventional NMR manipulations. Numerous composite pulses have been proposed to date in the context of QIP [10,16–23].

Geometric quantum computation [24,25] has been proposed to attain reliable quantum control. In addition to the dynamical phase, cyclic evolution of a quantum system allows for various geometric phases [26–30], which are controllable and thereby can be used for unitary operations. Hereafter, we call a gate implemented with a geometric phase a geometric quantum gate (GQG). Mathematically, a geometric phase is regarded as a holonomy associated with a closed path in a suitable base manifold associated with a cyclic evolution [31–33]. Random fluctuations along the integration path are expected to cancel out, leading to a quantum gate robust against random noise. Although there is numerical support for the robustness of GQGs [34], this issue is still under debate [35].

In this study, we unite these two apparently different constructions of robust unitary operations. More precisely, we reveal that composite pulses robust against certain kinds of systematic errors are nothing but GQGs. This has been observed previously in one-qubit operations [36]. Now we elaborate and generalize this observation to two-qubit operations that are indispensable for a universal set of quantum gates in QIP. Our work reveals that many composite pulses are geometric in nature, and their robustness is attributed to the robustness of GQGs against certain errors.

This study is organized as follows. Geometric phase—in particular, the Aharonov–Anandan phase—and its application to the implementation of a quantum gate are introduced in §2. We use perturbation theory as a guiding principle to design composite pulses and derive the robustness condition in §3. In §4, we present the main statement of this study—that is, existing composite pulses to suppress the pulse length error and the $J$-coupling error are GQGs. We will use a group theoretical argument to present our statement in a unified manner. The assertion in §4 is exemplified in §§5 and 6 by analysing various composite pulses from our viewpoint. Section 7 is devoted to a conclusion and discussions.

2. Geometric quantum gates

Geometric phase, anticipated in many branches of physics and chemistry [26], was formulated first by Berry in an adiabatic evolution of a quantum system. Berry [27] considered a cyclic evolution of a quantum system whose Hamiltonian has time-dependent parameters, and pointed out that after the cyclic and adiabatic evolution, the system may acquire not only the dynamical phase factor, but also a geometric phase factor that is given by a circuit integral in the parameter manifold. This integral is geometric, in the sense that it is independent of how fast the circuit is traversed. The Berry phase has been generalized in many ways. One such generalization is the Wilczek–Zee holonomy. In the presence of $n$-fold degeneracy, the geometric phase factor can be replaced by an element of a unitary group $U(n)$, which is also independent of how fast the circuit is traversed [28].

Aharonov & Anandan [29] showed that the geometric phase appears, even in non-adiabatic evolution. Consider an $n$-level system, whose normalized state
vector at time $t \in [0, T]$ is given by $|\psi(t)\rangle \in \mathbb{C}^n$. The dynamics of the system is characterized by the Schrödinger equation

$$i\frac{d}{dt}|\psi(t)\rangle = H(\lambda(t))|\psi(t)\rangle,$$  \hspace{1cm} (2.1)

where the Hamiltonian $H(\lambda(t))$ is Hermite and time-dependent through parameters $\lambda(t) = (\lambda_1(t), \ldots, \lambda_N(t))$. Here, we set $\hbar = 1$. When the evolution is cyclic with a period $T$, i.e.

$$|\psi(T)\rangle = e^{i\gamma}|\psi(0)\rangle, \quad \gamma \in \mathbb{R},$$  \hspace{1cm} (2.2)

then the phase $\gamma$ that the system acquires after the cyclic evolution includes the geometric contribution $\gamma_g$, which is defined in terms of the dynamical phase $\gamma_d$ as follows:

$$\gamma_g = \gamma - \gamma_d, \quad \gamma_d = -\int_0^T dt \langle \psi(t)|H(\lambda(t))|\psi(t)\rangle.$$  \hspace{1cm} (2.3)

This phase $\gamma_g$ is called the Aharonov–Anandan phase. It is possible to interpret the Aharonov–Anandan phase in terms of the geometrical structure of the Hilbert space $\mathbb{C}^n$. See appendix A, for details. In addition, for another expression of the Aharonov–Anandan phase, see earlier studies [29, 30, 33].

Applications of geometric phases are found in QIP. For example, Zanardi & Rasetti [24] proposed to use the Wilczek–Zee holonomy to implement unitary gates. It is also possible to implement unitary gates by using the Aharonov–Anandan phase [10, 25, 36–38]. To see this, let $\{|\psi_a\rangle\}_{1 \leq a \leq n}$ be the eigenvectors of a Hamiltonian $H(\lambda(0))$ and suppose their dynamical evolution is cyclic, that is,

$$|\psi_a(T)\rangle = U(T)|\psi_a\rangle, \quad U(T) = T \ e^{-i\int_0^T ds H(\lambda(s))}$$  \hspace{1cm} (2.4)

and

$$|\psi_a(T)\rangle = e^{i\gamma^a}|\psi_a\rangle, \quad \gamma^a \in \mathbb{R},$$  \hspace{1cm} (2.5)

where the time-ordered product is denoted by $T$. Equating equations (2.5) and (2.4), we observe that $|\psi_a\rangle$ is an eigenvector of $U(T)$ with the eigenvalue $e^{i\gamma^a}$, that is,

$$U(T)|\psi_a\rangle = e^{i\gamma^a}|\psi_a\rangle.$$  \hspace{1cm} (2.6)

When there is no degeneracy, the spectral decomposition of $U(T)$ is written as

$$U(T) = e^{i\gamma_1}|\psi_1\rangle \langle \psi_1| + \cdots + e^{i\gamma_n}|\psi_n\rangle \langle \psi_n|.$$  \hspace{1cm} (2.7)

The phase $\gamma^a$ is decomposed as $\gamma^a = \gamma_g^a + \gamma_d^a$, where $\gamma_d^a$ is the dynamical phase defined as

$$\gamma_d^a = -\int_0^T dt \langle \psi_a(t)|H(\lambda(t))|\psi_a(t)\rangle \quad \text{and} \quad |\psi_a(t)\rangle = U(t)|\psi_a\rangle.$$  \hspace{1cm} (2.8)

A unitary operator $U(T)$ is called a GQG, if $\gamma_d^a$ vanishes for all $a$.

3. Perturbative construction of composite pulses

In actual situations in NMR, the dynamics is controlled by a sequential application of radiofrequency (RF) pulses with constant field strength.

Phil. Trans. R. Soc. A (2012)
Accordingly, the time interval $[0, T]$ is divided into $k$ intervals, in each of which the Hamiltonian is constant. More precisely, we define the $i$th temporal interval $[t_{i-1}, t_i]$, where $t_i$ satisfies $0 = t_0 < t_1 < \cdots < t_k = T$, and define a piecewise constant Hamiltonian that takes the form $H(\lambda^i)$ in the $i$th interval $[t_{i-1}, t_i]$. Here, $\lambda^i = (\lambda_1^i, \ldots, \lambda_N^i)$ is a constant parameter vector, whereas $N$ is the number of control parameters. Then, the $i$th RF pulse gives rise to a unitary operator

$$e^{-iW^i}, \quad W^i = H(\lambda^i) \cdot (t_i - t_{i-1}), \quad (3.1)$$

and $U(T)$ can be written as

$$U(T) = e^{-iW^k} \cdots e^{-iW^1}. \quad (3.2)$$

Now we wish to implement a ‘target’ unitary operator $U$ as $U = U(T)$. The target $U$ should be implemented in a way that is robust against the error under consideration as much as possible. Hereafter, we seek a condition for such robust implementation.

We consider errors that cause displacement

$$W^i \rightarrow W^i + \delta W^i, \quad (3.3)$$

where $\delta W^i$ is a self-adjoint operator corresponding to the error. When $\delta W^i$ is sufficiently small in the sense of the operator norm, we can use the perturbation theory and find

$$e^{-i(W^i + \delta W^i)} \approx e^{-iW^i} (1_n - i\delta W^i) \quad \text{and} \quad \delta W^i := \int_0^1 dx e^{ixW^i} \delta W^i e^{-ixW^i}, \quad (3.4)$$

to the first order in $\delta W^i$. Here, the identity operator on $\mathbb{C}^n$ is denoted by $1_n$. The operator $\delta W^i$ is the error operator $\delta W^i$ in the interaction picture. Then, the unitary operator $U'$ implemented with the error $\delta W^i$ is given by

$$U' = e^{-i(W^k + \delta W^k)} \cdots e^{-i(W^1 + \delta W^1)} \approx U(1_n - i\Delta W), \quad (3.5)$$

where

$$\Delta W = \sum_{i=1}^k V^{i-1} \delta W^i V^{i-1}, \quad V^i = e^{-iW^i} \cdots e^{-iW^1} \quad \text{for} \ i = 1, 2, \ldots, k - 1, \quad (3.6)$$

with $V^0 = 1$. Many, although not all, composite pulses satisfy the following robustness condition:

$$\Delta W = 0, \quad (3.7)$$

which we can evaluate once we specify $\delta W^i$. This condition guarantees the effect of the error vanishing to the first order in $\delta W^i$.

Now, we wish to address the relation between the robustness condition (3.7) and a classification of composite pulses common in the NMR community. There are two types (type A and type B) of composite pulses [5,16]. The error tolerance is independent of the initial state vector for type A composite pulses, whereas it is not the case for type B composite pulses. In view of this, the composite pulses satisfying (3.7) are clearly of type A.
4. Composite pulses as geometric quantum gates

To see the geometric nature of type A composite pulses, we follow the argument introduced earlier [36], which has been generalized to a multi-qubit system in [10]. Suppose that the systematic error is proportional to $W^i$,

$$\delta W^i = \epsilon W^i. \quad (4.1)$$

As shown later, two kinds of systematic errors are of this form. The robustness condition (3.7) reads

$$\Delta W = \epsilon \sum_{i=1}^{k} V^{i-1\dagger} W^i V^{i-1} = 0, \quad (4.2)$$

where use has been made of the identity $\delta W^i = \delta W^i$ derived from equation (3.4) and equation (4.1). By taking the expectation value of $\Delta W$ with respect to $|a\rangle$, we obtain

$$\gamma_a = \sum_{i=1}^{k} \gamma_a(i) = 0 \quad \text{and} \quad \gamma_a(i) := -\langle a(i-1)|W^i|a(i-1)\rangle, \quad (4.3)$$

where $|a(i)\rangle := V^i|a\rangle$. Hence, any composite pulse that is designed by the perturbation theory and compensates the error (4.1) is GQG. In what follows, we will show that composite pulses associated with two kinds of relevant systematic errors are GQGs.

(a) Error in the one-qubit system

We turn to a one-qubit system, whose Hilbert space is $\mathbb{C}^2$. A special unitary group 2 (SU(2)) operation that we can implement with a single RF pulse in NMR is limited to the following form:

$$W^i = \theta_i \cdot \frac{\sigma}{2}, \quad (4.4)$$

where $n_i = (\cos \phi_i, \sin \phi_i, 0)$ and $\sigma = (\sigma_x, \sigma_y, \sigma_z)$ owing to the apparatus limitation. Nevertheless, we can implement any SU(2) operation by combining at most three such pulses using the Euler angle decomposition [12,15]. The displacement (3.3) under the error (4.1) is seen as

$$\theta_i \rightarrow (1 + \epsilon)\theta_i. \quad (4.5)$$

This is a well-known systematic error called the pulse length error in the NMR community [5]. Hence, from the previous argument, we observe that any composite pulse compensating for the pulse length error is a GQG.

(b) Error in the two-qubit system

For a two-qubit system, the relevant Hilbert space and the set of unitary operations are $\mathbb{C}^2 \otimes 2$ and SU(4), respectively. In view of QIP, the CNOT operation

$$U_{\text{CNOT}} = |0\rangle\langle 0| \otimes 1_2 + |1\rangle\langle 1| \otimes \sigma_x \quad (4.6)$$
is important.\textsuperscript{1} Here, $|a\rangle \in \mathbb{C}^2$ with $a = 0, 1$ is the eigenvector of $\sigma_z$ with the eigenvalue $(-1)^a$. The relevance of the CNOT operation originates from the fact that any QIP can be implemented as a quantum circuit composed of one-qubit unitary operations and CNOT operations \cite{11,12,15}.

By using the Cartan decomposition \cite{15}, the CNOT operation can be rewritten as $U_{\text{CNOT}} = K_1 HK_2$, with

$$H = e^{i\alpha_2 \sigma_z \otimes \sigma_z} e^{i\alpha_1 \sigma_y \otimes \sigma_y} e^{i\alpha_3 \sigma_z \otimes \sigma_z} \quad \text{and} \quad K_1, K_2 \in SU(2) \otimes SU(2). \quad (4.7)$$

Because $\sigma_x \otimes \sigma_x$ is generated from $\sigma_z \otimes \sigma_z$ through the following identity:

$$e^{i\alpha_2 \sigma_z \otimes \sigma_z} = e^{i\pi(\sigma_y \otimes \mathbb{1}_2 + \mathbb{1}_2 \otimes \sigma_y)/4} e^{i\alpha_2 \sigma_z \otimes \sigma_z} e^{-i\pi(\sigma_y \otimes \mathbb{1}_2 + \mathbb{1}_2 \otimes \sigma_y)/4}, \quad (4.8)$$

the Ising-type Hamiltonian

$$H = \frac{J}{4} \sigma_z \otimes \sigma_z \quad (4.9)$$

is essential to implement CNOT operations, which is commonly realized in a weak coupling limit. Hereafter, we shall be concerned with the $J$-coupling error defined by

$$J \rightarrow (1 + \epsilon)J. \quad (4.10)$$

Several composite pulses robust against the $J$-coupling error have been proposed, assuming that one-qubit operations are free from errors. These existing composite pulses \cite{17–20} are designed by making use of the following three generators only:

$$X := \sigma_z \otimes \sigma_z, \quad Y := \sigma_z \otimes \sigma_x \quad \text{and} \quad Z := \mathbb{1}_2 \otimes \sigma_y, \quad (4.11)$$

among the 15 generators of SU(4). Evidently, these operators satisfy $su(2)$ algebra,

$$\begin{bmatrix} X & \frac{Y}{2} \end{bmatrix} = \frac{iZ}{2}, \quad \begin{bmatrix} \frac{Y}{2} & Z \end{bmatrix} = \frac{iX}{2} \quad \text{and} \quad \begin{bmatrix} Z & X2 \end{bmatrix} = \frac{iY}{2}. \quad (4.12)$$

Thus, we can construct an SU(2) subgroup by exponentiating the generators (4.11). Let us denote this subgroup by $G$.

Now, let us put

$$Q_i = \frac{J(t_i - t_{i-1})}{2}$$

and

$$W^i = \frac{Q_i(\cos \phi_i X + \sin \phi_i Y)}{2} = e^{-i\phi_i Z/2} \left( \frac{Q_i X}{2} \right) e^{i\phi_i Z/2}. \quad (4.13)$$

Then, we observe that

$$e^{-iW^i} = e^{-i\phi_i Z/2} e^{-iQ_iX/2} e^{i\phi_i Z/2} \in G. \quad (4.14)$$

Thus, for this $W^i$, we observe the identification between $Q_i, X, Y$ and $Z$ and $\theta_i, \sigma_x, \sigma_y$ and $\sigma_z$ in equation (4.4), respectively. Because the $J$-coupling error (4.10) is equivalent to the pulse length error (4.5) under this identification, we can

\textsuperscript{1}Precisely speaking, $\det U_{\text{CNOT}} = -1$ and it is not an element of SU(4). Nevertheless, we can multiply this matrix by an unphysical phase $e^{i\pi/4}$ to make it an element of SU(4). Two quantum gates that differ by an overall phase will be identified hereafter.

*Phil. Trans. R. Soc. A* (2012)
construct a ‘composite pulse’, which is robust against the $J$-coupling error, if we merely replace $\theta_i, \sigma_x, \sigma_y$ and $\sigma_z$ by $\Omega_i, X, Y$ and $Z$, respectively. In fact, as stated earlier, such composite pulses based on the identification have been proposed in earlier studies [17–20]. One of these composite pulses shall be examined later. Composite pulses designed under this identification are GQGs because this identification keeps the mathematical structure of the theory unchanged.

Two remarks are in order. First, the definition of $Z$ tells us that we can freely tune the parameter $\phi_i$ by changing the RF field along the $y$-axis of the second qubit. Second, if there exists $U \in G$ such that

$$U|\psi\rangle = e^{i\gamma}|\psi\rangle,$$

(4.15)

then the $G$-orbit $G|\psi\rangle$ of $|\psi\rangle$ is identified with $S^2$, which corresponds to the Bloch sphere regarded as the orbit of one-qubit operations on a single qubit. This observation ensures that we can visualize the time evolution of a cyclic state associated with $U \in G$ as a trajectory on the ‘Bloch’ sphere, as long as we use the composite pulses proposed so far.

5. Examples of geometric composite pulse

In this section, we give several examples demonstrating our claim that two types of composite pulses introduced in the previous section are GQGs. To this end, we shall evaluate the dynamical phase of several composite pulses and verify that the dynamical phase indeed vanishes in all cases.

(a) The one-qubit system

We parametrize our target $U$ as

$$U = \exp(-i\theta n \cdot \sigma/2) \quad \text{and} \quad n = (\cos \phi, \sin \phi, 0).$$

(5.1)

Then, from §2, a cyclic state $|\psi_a\rangle$ associated with $U$ is given as an eigenvector of $U$, that is,

$$|\psi_a\rangle = |(-1)^a n\rangle, \quad a = 0, 1,$$

(5.2)

where $|(-1)^a n\rangle$ is the eigenstate of $n \cdot \sigma$ such that

$$n \cdot \sigma|(-1)^a n\rangle = (-1)^a|(-1)^a n\rangle.$$

(5.3)

We shall often use the following useful formula:

$$\langle n|m \cdot \sigma|n\rangle = n \cdot m.$$

(5.4)

Note that the vector $n$ is the Bloch vector for the state $|n\rangle$ and we have

$$U|(-1)^a n\rangle = \omega_a|(-1)^a n\rangle \quad \text{and} \quad \omega_a = \exp\left[\frac{(-1)^a+1i\theta}{2}\right].$$

(5.5)

All composite pulses, for which we evaluate the dynamical phases, are composed from $k = 2l - 1$ pulses, which satisfy the ‘time-symmetric’ condition

$$W^i = W^{k+1-i}.$$

(5.6)
Many implications of this condition are found in Levitt [5]. Now we address that this condition leads to

$$\gamma^a_d(i) = \gamma^a_d(k + 1 - i).$$

(5.7)

See appendix B for the proof. Hence, the dynamical phase is rewritten as

$$\gamma^a_d = 2[\gamma^a_d(1) + \ldots + \gamma^a_d(l - 1)] + \gamma^a_d(l)$$

(5.8)

for a composite pulse, which is made of $k = 2l - 1$ pulses.

(i) $90^\circ-180^\circ-90^\circ$ pulse

The first composite pulse was proposed by Levitt & Freeman [4] based on a trajectory on the Bloch sphere. This is a $k = 3$ symmetric composite pulse defined by

$$\begin{align*}
\theta_1 &= \frac{\theta_2}{2} = \theta_3 = \frac{\pi}{2}, & \phi_1 = \phi_3 &= 0,
\phi_2 &= \frac{\pi}{2}.
\end{align*}$$

(5.9)

We immediately find

$$W_1 = W_3 = \frac{\pi}{4}\hat{x} \cdot \sigma \quad \text{and} \quad W_2 = \frac{\pi}{2}\hat{y} \cdot \sigma,$$

(5.10)

which leads to

$$U = e^{-iW_1}e^{-iW_2}e^{-iW_1} = -i\sigma_y.$$  

(5.11)

Hence, we observe that the target is fixed to $q = \frac{\pi}{4}$ and $f = \frac{\pi}{2}$, and there are no free parameters we may adjust. It follows from equation (5.11) that $|\psi_a) = |(1)^a\hat{y}\rangle$.

Let us proceed to the calculation of the dynamical phase. First, we have

$$\gamma^a_d(1) = -\frac{\pi}{4}|(1)^a\hat{y}|\begin{pmatrix} \hat{x} \cdot \sigma \end{pmatrix}(-1)^a\hat{y}) = (-1)^a+1\frac{\pi}{4}\hat{x} \cdot \hat{y} = 0$$

(5.12)

from formula (5.4). Next, we observe

$$|\psi_a(1)) = e^{-iW_1}|\psi_a) = e^{-i\pi\sigma_y/4}|(1)^a\hat{y}) = |(1)^a\hat{z})$$

(5.13)

to obtain

$$\gamma^a_d(2) = -\frac{\pi}{2}|(1)^a\hat{y}|\begin{pmatrix} \hat{y} \cdot \sigma \end{pmatrix}(-1)^a\hat{z}) = (-1)^a+1\frac{\pi}{2}\hat{y} \cdot \hat{z} = 0.$$  

(5.14)

Summing up these, we reach

$$\gamma^a_d = 2\gamma^a_d(1) + \gamma^a_d(2) = 0.$$  

(5.15)

We can confirm equation (5.7) by further calculation. We find

$$|\psi_a(2)) = e^{-iW_2}e^{-iW_1}|\psi_a) = e^{-iW_2}|(1)^a\hat{z}) = |(1)a+1\hat{z}),$$

(5.16)

from which it follows that

$$\gamma^a_d(3) = -\frac{\pi}{4}|(1)^{a+1}\hat{z}|\begin{pmatrix} \hat{x} \cdot \sigma \end{pmatrix}(-1)^{a+1}\hat{z}) = (-1)^a\frac{\pi}{4}\hat{x} \cdot \hat{z} = 0 = \gamma^a_d(1).$$  

(5.17)

The time evolution of the cyclic states ends up with

$$|\psi_a(3)) = e^{-iW_3}|\psi_a(2)) = |(1)^a\hat{y}) = |\psi_a),$$

(5.18)
as expected. These results are summarized as

$$|\pm \hat{y}\rangle \xrightarrow{e^{-iW_1}} |\pm \hat{z}\rangle \xrightarrow{e^{-iW_2}} |\mp \hat{z}\rangle \xrightarrow{e^{-iW_3}} |\pm \hat{y}\rangle$$

and $\gamma_d^a(i) = 0$. (5.19)

For the graphical representation of this excursion, see figure 1.

The lesson we learn from this composite pulse is that the converse of our statement is not always true: not all GQGs for a spin-1/2 system are type A composite pulses that are robust against the pulse length error. Indeed, this pulse is of type B because $\Delta W \neq 0$. This has been overlooked in Kondo & Bando [36].

(ii) Short composite rotation for undoing length over and under shoot (SCROFULOUS)

SCROFULOUS is a $k = 3$ time-symmetric composite pulse constructed by Cummins et al. [21]. This composite pulse was designed by using perturbation theory and quaternion algebra. Given a target (5.1), SCROFULOUS takes the following form:

$$\begin{aligned}
\theta_1 &= \theta_3 = \text{arcsinc} \left[ \frac{2 \cos(\theta/2)}{\pi} \right], \\
\theta_2 &= \pi, \\
\phi_1 &= \phi_3 = \phi + \text{arccos} \left[ \frac{\pi \cos \theta_1}{2\theta_1 \sin(\theta/2)} \right], \\
\phi_2 &= \phi_1 - \text{arccos} \left[ \frac{\pi}{2\theta_1} \right],
\end{aligned}$$

(5.20)

where sinc $x = \sin x/x$. Note that SCROFULOUS implements any one-qubit unitary operator of the form (5.1).
Let us evaluate the dynamical phase. We set $\phi = 0$ for simplicity, while extension to an arbitrary $\phi$ is straightforward. First, we have

$$
\gamma^a_1 = -\theta_1 ((-1)^a n_1 \cdot \sigma / 2) ((-1)^a n_1 / 2) = (-1)^{a+1} \theta_1 n_1 \cdot n_1 / 2
$$

Next, observe that

$$
V^1 W^2 V^1 = \frac{\theta_2}{2} \left[ \cos^2 \left( \frac{\theta_1}{2} \right) n_2 + \sin^2 \left( \frac{\theta_1}{2} \right) m - \sin \theta_1 (n_1 \times n_2) \right] \cdot \sigma, \quad (5.22)
$$

where

$$
m = 2(n_2 \cdot n_1) n_1 - n_2. \quad (5.23)
$$

Because we have

$$
n_2 \cdot n = \cos \phi_2 = -\frac{\pi \cos \phi_1}{2\theta_1} + \sin \phi_1 \sin \left[ \arccos \left( \frac{-\pi}{2\theta_1} \right) \right],
$$

$$
m \cdot n = \cos(2\phi_1 - \phi_2) = -\frac{\pi \cos \phi_1}{2\theta_1} - \sin \phi_1 \sin \left[ \arccos \left( \frac{-\pi}{2\theta_1} \right) \right] \quad (5.24)
$$

and $(n_1 \times n_2) \cdot n = 0$,

we observe

$$
\gamma^a_2 = -\langle \psi_a | V^1 W^2 V^1 | \psi_a \rangle
$$

$$
= (-1)^a \left( \frac{\pi}{2} \right) \left\{ \left( \frac{\pi}{2\theta_1} \right) \cos \phi_1 + \cos \theta_1 \sin \left[ \arccos \left( \frac{-\pi}{2\theta_1} \right) \right] \sin \phi_1 \right\}. \quad (5.25)
$$

Using $\sin(\arccos x) = \sqrt{1 - x^2}$ and

$$
\sin \phi_1 = \frac{\sqrt{1 - \left( \pi/(4\theta_1) \right)^2}}{\sin(\theta/2)}, \quad (5.26)
$$

we immediately derive

$$
\gamma^a = 2\gamma^a_1 + \gamma^a_2
$$

$$
= (-1)^a \left\{ \theta_1 \left[ 1 - \left( \frac{\pi}{2\theta_1} \right)^2 \right] \cos \phi_1 
\right.
$$

$$\left. + (\pi/2) \cos \theta_1 \sin \left[ \arccos \left( \frac{-\pi}{2\theta_1} \right) \right] \sin \phi_1 \right\}
$$

$$
= (-1)^a \left[ 1 - \left( \frac{\pi}{2\theta_1} \right)^2 \right] \left[ \theta_1 \cos \phi_1 + \frac{\pi \cos \theta_1}{2 \sin(\theta/2)} \right]
$$

$$
= 0. \quad (5.27)
$$

Hence, SCROFULOUS is a GQG. The trajectory of the cyclic state is given in figure 2.

Phil. Trans. R. Soc. A (2012)
Figure 2. Excursion of the cyclic state $|\hat{x}\rangle$ of the SCROFULOUS for a target $\theta = \pi$, $\phi = 0$ on the Bloch sphere. The large arrow is the Bloch vector of the cyclic state. The state $e^{-iW^1}|\hat{x}\rangle$ pauses during the application of the pulse $W^2$ because it is an eigenstate of the pulse $W^2$. The solid angle of the shaded area is equal to $\theta$; this composite pulse is a GQG. (Online version in colour.)

(iii) **Broad band 1**

Now we turn to the broad band 1 (BB1), which was proposed by Wimperis [39]. For the sake of simplicity, we treat a $k=5$ time-symmetric variant of the BB1 sequence. We call this variant time-symmetric BB1. The BB1 pulse sequence is useful for the implementation of QIP because it compensates for the pulse length error up to second order in the perturbative expansion [16]. There are two techniques to generalize the BB1 pulse sequence [22]. By using these techniques, we can design a composite pulse sequence that compensates for the pulse length error up to an arbitrary higher order in perturbative expansion.

For a target (5.1) with angles $\theta$ and $\phi$, the time-symmetric BB1 consists of

$$
\begin{align*}
\theta_1 &= \theta_5 = \frac{\theta}{2}, & \theta_2 &= \frac{\theta_3}{2} = \theta_4 = \pi, \\
\phi_1 &= \phi_5 = \phi, & \phi_2 &= \phi_4 = \phi + k \quad \text{and} \quad \phi_3 = 3\phi + k,
\end{align*}
$$

(5.28)

with

$$
\kappa = \arccos \left[ -\frac{\theta}{4\pi} \right].
$$

(5.29)

Let us evaluate the dynamical phase associated with the time-symmetric BB1. First, we note from $U = e^{-2iW^1}$ that

$$
V^1|\psi_a\rangle = e^{-iW^1}|\psi_a\rangle = \pm \sqrt{\omega_a}|\psi_a\rangle.
$$

(5.30)

Then, we have

$$
\gamma^a_d(1) = -\langle \psi_a | W^1 | \psi_a \rangle = \frac{(-1)^{a+1} \theta_1 \cdot n_1 \cdot n}{2} = \frac{(-1)^{a+1} \theta}{4}.
$$

(5.31)
Next, we find from $\theta_2 = \pi$ and $\phi_2 = \phi + \kappa$ that
\[
\gamma_{d}^a(2) = -(\psi_a|V_1 W_2^2 \psi_a)^2 = -(\psi_a|W_2^2 \psi_a) = \frac{(-1)^{a+1} \pi n_2 \cdot n}{2} = \frac{(-1)^a \theta}{8},
\]
\[
e^{-i W_2^2 |\psi_a} = |(-1)^a n'\rangle \quad \text{and} \quad n' = (\cos(\phi + 2\kappa), \sin(\phi + 2\kappa), 0).
\]
This leads to
\[
\gamma_{d}^a(3) = -(\psi_a|V_2^2 W_2^2 \psi_a) = (-1)^{a+1} \pi n_3 \cdot n' = (\frac{(-1)^a \theta}{4}).
\]
By adding individual dynamical phases, we finally obtain
\[
\gamma_{d}^a = 2\gamma_{d}^a(1) + 2\gamma_{d}^a(2) + \gamma_{d}^a(3) = (\frac{(-1)^a \theta}{4}).
\]
This result confirms that the time-symmetric BB1 is also a GQG.

(iv) Knill’s sequence

Knill’s sequence [40,41] is a $k = 5$ time-symmetric composite pulse. This sequence implements the target $U$ given by
\[
\theta = \pi \quad \text{and} \quad n = \left(\cos\left(\frac{\alpha - \pi}{6}\right), \sin\left(\frac{\alpha - \pi}{6}\right), 0\right).
\]
where $\alpha$ is a free parameter. The sequence is defined by
\[
\theta_i = \pi \quad (1 \leq i \leq 5), \quad \phi_1 = \phi_5 = \alpha + \frac{\pi}{6}, \quad \phi_2 = \phi_4 = \alpha \quad \text{and} \quad \phi_3 = \alpha + \frac{\pi}{2}.
\]
This sequence is used in experiments to maintain the coherence of nitrogen-vacancy centres in diamond [40] and to decouple a system from the environment [41]. Note that this sequence is robust against not only the pulse length error, but also the off-resonance error [41].

Let us calculate the dynamical phase. First, we have
\[
\gamma_{d}^a(1) = -(\psi_a|W_1 \psi_a) = \frac{(-1)^{a+1} \pi n_1 \cdot n}{2} = (\frac{-1)^a \theta}{4})
\]
We find $\gamma_{d}^a(2)$ with
\[
\gamma_{d}^a(2) = 0.
\]
Further, we observe $\gamma_{d}^a(3)$ with
\[
\gamma_{d}^a = 2\gamma_{d}^a(1) + 2\gamma_{d}^a(2) + \gamma_{d}^a(3).
\]
This result confirms that the time-symmetric BB1 is also a GQG.
Then, we have
\[ \gamma_d^a(3) = (-1)^a \frac{\pi}{2}. \] (5.42)

We find that, by adding individual dynamical phases,
\[ \gamma_d^a = 2\gamma_d^a(1) + 2\gamma_d^a(2) + \gamma_d^a(3) = (-1)^{a+1} \left( \frac{\pi}{2} + 0 - \frac{\pi}{2} \right) = 0. \] (5.43)

This example shows that the composite pulses robust against several systematic errors are also GQGs, if they compensate for at least the pulse length error. Thus, by construction, the composite pulses proposed in earlier studies \[10,23\], which are simultaneously robust against the above two errors, are also GQGs.

\( b \) The two-qubit system

Because our interest lies in the CNOT operation, we choose the target
\[ U = e^{-i\omega X/2}, \] (5.44)
which is the entangling part in the CNOT gate. The cyclic state \( |\psi_a\rangle \) is an eigenstate of \( X \) in equation (4.11). In the binary notation \( a = 2p + q \), where \( p, q \in \{0,1\} \), we find
\[ |\psi_a\rangle = |p\rangle \otimes |q\rangle. \] (5.45)

Jones designed a composite pulse sequence for a two-qubit system from a one-qubit composite pulse sequence \[17\], by employing isomorphism among the generators given in §4b. Let us introduce a notation \( (Q)_\phi = \exp[-i\phi X + \sin \phi Y]/2 \) and set the target to \( (\pi/2)_0 \) in this notation. Jones’s sequence is given by
\[ (\pi 4)_0(\pi)_k(2\pi)_3(\pi)_k(\pi 4)_0, \quad \kappa = \arccos \left( \frac{-1}{8} \right). \] (5.46)

Because the isomorphism maps \( X, Y \) and \( Z \) to the Pauli matrices \( \sigma_x, \sigma_y \) and \( \sigma_z \), respectively, Jones’s sequence is a two-qubit analogue of the BB1 sequence: the combination of the first and last pulses is the target pulse \( (\theta = \pi/2, \phi = 0) \) and the others are the same as the BB1 sequence (5.28). Similarly, the composite pulses in earlier studies \[18–20\] are the two-qubit counterparts of those in Brown et al. \[22\].

Evaluation of the dynamical phase is easy, if we make use of the already-mentioned isomorphism. Because \( X \) is mapped to \( \sigma_x \), the cyclic vector \( |p\rangle \otimes |q\rangle \) should be sent to \( |(1)^{p+q}\sigma_x\rangle \), which is also an eigenvector of the target \( U = \exp(-i\pi \sigma_x/4) \). Thus, the dynamical phase of Jones’s sequence is transferred to that of the BB1 sequence, which leads to
\[ \gamma_d^a = 0, \] (5.47)
showing the sequence has a vanishing dynamical phase. One can also achieve the same result by direct calculation without employing the isomorphism.

Phil. Trans. R. Soc. A (2012)
6. Two composite z-rotations

In NMR, rotations around the z-axis must be implemented by a sequence of pulses because the RF pulses (4.4) have the restriction \( \vec{n}_i \perp \hat{z} \). Thus, it is of interest to investigate whether the sequences are geometric.

First, we consider the following \( k = 3 \) sequence to realise a target \( U = e^{-i\theta z/2} \):

\[
\theta_1 = \theta_3 = \frac{\pi}{2}, \quad \theta_2 = \theta, \quad \phi_1 = -\phi_3 = \frac{\pi}{2} \quad \text{and} \quad \phi_2 = 0. \tag{6.1}
\]

The cyclic states are \( |\psi_a\rangle = |(-1)^a \hat{z}\rangle = |a\rangle \). Let us calculate the dynamical phase. The first one is

\[
\gamma_d^a(1) = -\frac{\pi}{4} \langle \psi_a | \hat{y} \cdot \sigma | \psi_a \rangle = (-1)^{a+1} \frac{\pi}{4} \hat{y} \cdot \hat{z} = 0. \tag{6.2}
\]

We find \( V^1|\psi_a\rangle = |(-1)^a \hat{x}\rangle \), which leads to

\[
\gamma_d^a(2) = -\frac{\theta}{2}((-1)^a \hat{x} | \hat{x} \cdot \sigma | (-1)^a \hat{x}) = (-1)^{a+1} \frac{\theta}{2}. \tag{6.3}
\]

Furthermore, we obtain \( V^2|\psi_a\rangle = \exp((-1)^{a+1}i\theta/2) |(-1)^a \hat{x}\rangle \). Thus, we observe

\[
\gamma_d^a(3) = \frac{\pi}{4}((-1)^a \hat{x} | \hat{y} \cdot \sigma | (-1)^a \hat{x}) = (-1)^a \frac{\pi}{4} \hat{y} \cdot \hat{x} = 0. \tag{6.4}
\]

We conclude

\[
\gamma_d^a = (-1)^{a+1} \frac{\theta}{2} \neq 0. \tag{6.5}
\]

Hence, the pulse sequence (6.1) is not a GQG. Note that this sequence is not robust against the pulse length error, that is, \( \Delta W \neq 0 \), which is exactly the contraposition of our claim.

Second, we investigate a \( k = 2 \) pulse for \( U = e^{i\theta z/2} \),

\[
\theta_1 = \theta_2 = \pi, \quad \phi_1 = 0 \quad \text{and} \quad \phi_2 = \frac{\theta}{2}. \tag{6.6}
\]

The cyclic states are the same as those of the previous sequence. We have

\[
\gamma_d^a(1) = -\frac{\pi}{2} \langle \psi_a | \hat{x} \cdot \sigma | \psi_a \rangle = (-1)^{a+1} \frac{\pi}{2} \hat{x} \cdot \hat{z} = 0. \tag{6.7}
\]

By the same way, we compute

\[
\gamma_d^a(2) = 0, \tag{6.8}
\]

which clearly shows

\[
\gamma_d^a = 0. \tag{6.9}
\]

Hence, the pulse sequence (6.6) is a GQG. This pulse is, however, not robust against the pulse length error. Indeed, we may check

\[
\Delta W = e^{\frac{\pi}{2}} \left[ \left( 1 + \cos \frac{\theta}{2} \right) \sigma_x - \sin \frac{\theta}{2} \sigma_y \right] \neq 0 \tag{6.10}
\]

Phil. Trans. R. Soc. A (2012)
Figure 3. Excursions of the cyclic states on the Bloch sphere. (a) The trajectory of the cyclic state $|\hat{z}\rangle$ under the pulse sequence (6.1). Note that the trajectory fails to close, which shows that this sequence is dynamical. (b) The trajectory of the cyclic state $|-\hat{z}\rangle$ under the pulse sequence (6.6) for $\theta = \pi$. The solid angle subtended by the trajectory of the Bloch vector is $\pi = \theta$, which shows the geometric nature of the sequence. (Online version in colour.)

by direct calculation. This also tells us that not all GQGs are robust against the pulse length error. The difference of these two composite $z$-rotations are visualized in figure 3.

7. Conclusion and discussions

In this study, we uncovered the relation between GQGs and the composite pulses robust against certain kinds of systematic errors. For the error (4.1), proportional to the Hamiltonian times the operation time, the compensation of the error automatically leads to a vanishing dynamical phase. Thus, a non-trivial operation by a composite pulse robust against such an error is a GQG.

We pointed out that there are two kinds of errors assuming the form (4.1). One is the pulse length error, and the other is the $J$-coupling error. This implies that the composite pulses robust against these errors are GQGs. This observation was illustrated and confirmed by directly showing that the dynamical phase vanishes for several typical composite pulses: $90^\circ$–$180^\circ$–$90^\circ$, SCROFULOUS, BB1, Knill’s sequence for the pulse length error and Jones’s pulse sequence for the $J$-coupling error. The two most common composite $z$-rotations were also examined.

Our work has shown that we can construct a universal gate set composed of GQGs simply by using the composite pulses. This suggests that NMR is quite a useful test bench of geometric quantum computation. In view of this, further study of composite pulses, for example Ota & Kondo [37], is desirable for a deeper understanding of the geometric quantum computation.

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Phil. Trans. R. Soc. A (2012)
Figure 4. Schematic of the Aharonov–Anandan phase. The set of the normalized states forms $S^{2n-1} \subset \mathbb{C}^n$, and this subset $S^{2n-1}$ can be seen as a $U(1)$-bundle over the projective Hilbert space $\mathbb{C}P^{n-1}$. Given a closed path in the base manifold $\mathbb{C}P^{n-1}$, the horizontal lift of the path is naturally defined by a connection in the $U(1)$-bundle. The holonomy associated with the horizontal lift is given as $e^{i\gamma} \in U(1)$, which can be seen as a global phase difference accumulated through the parallel transport along the horizontal lift on the path in $\mathbb{C}P^{n-1}$.

Appendix A. Geometry of the Aharonov–Anandan phase

Here, we outline the relevant aspects of the Aharonov–Anandan phase in the context of the present study. The geometrical nature of the Aharonov–Anandan phase is derived from that of the fibre bundle structure associated with the Hilbert space. See earlier studies [13,32] for technical details.

Consider the Hilbert space $\mathbb{C}^n$. In quantum mechanics, we are exclusively concerned with the set of normalized vectors in $\mathbb{C}^n$. The set of normalized vectors form the $(2n-1)$-dimensional sphere $S^{2n-1} \subset \mathbb{C}^n$. Moreover, we need to identify vectors that differ by an overall phase; two normalized states $|\psi\rangle$ and $e^{i\gamma}|\psi\rangle$ represent the identical physical state for any $\gamma \in \mathbb{R}$. The manifold obtained from $S^{2n-1}$ under this identification is called the complex projective space,

$$\mathbb{C}P^{n-1} \simeq S^{2n-1}/U(1),$$

where $U(1)$ is the set of overall phases.

For $n = 2$, we obtain $\mathbb{C}P^1 = S^2$, which corresponds to the Bloch sphere. Accordingly, $S^3$ is identified with a $U(1)$-bundle over $S^2$ (the Hopf fibration). More generally, $S^{2n-1}$ is a $U(1)$-bundle over the base manifold $\mathbb{C}P^{n-1}$. A point in $\mathbb{C}P^{n-1}$ represents a physical state and its phase freedom is represented by the fibre $U(1)$. The identification naturally introduces the projection $\pi : S^{2n-1} \to \mathbb{C}P^{n-1}$. Fixing the phase is equivalent to taking a point in the fibre (figure 4).

It should be noted that $\mathbb{C}P^{n-1}$ has a natural metric called the Fubini–Study metric. Given a metric in the base manifold, we can construct a connection in the base manifold. This defines the horizontal lift of a given curve in the base manifold to the fibre bundle $S^{2n-1}$. Now suppose that there is a closed loop in the base

*Phil. Trans. R. Soc. A (2012)*
manifold. If one carries a point on a fibre over $p \in \mathbb{C}P^{n-1}$ along the horizontal lift of the loop, the point comes back to a point in the same fibre, which is not necessary the initial point. This $U(1)$ phase factor obtained after traversing a loop is called the holonomy associated with the loop and the horizontal lift. The Aharonov–Anandan phase is nothing but this $U(1)$ phase factor, which is geometric in the sense that it depends only on the loop in the base manifold and the connection of the $U(1)$-bundle but not on how fast the loop is traversed.

We note that twice the Aharonov–Anandan phase is the solid angle at the origin subtended by the trajectory of a state vector on the Bloch sphere ($\mathbb{C}P^1$, in this case) during a one-qubit operation.

**Appendix B. Proof of equation (5.7)**

Here, we prove equation (5.7). For this purpose, we first note the identity

$$\sigma_z W^i \sigma_z = -W^i$$  \hspace{1cm} (B.1)

for $W^i$ of equation (4.4) because $n_i \perp \hat{z}$. Multiplying by $-i$ and exponentiating equation (B.1), we find

$$\sigma_z e^{-iW^i} \sigma_z = e^{iW^i}. \hspace{1cm} (B.2)$$

Then, we obtain

$$V^{k-i} = e^{iW^i} \cdots e^{iW^1} U = \sigma_z V^i \sigma_z U \hspace{1cm} (B.3)$$

for a time-symmetric composite pulse. It then follows that

$$|\psi_a(k-i)\rangle = V^{k-i}|\psi_a\rangle = \sigma_z V^i \sigma_z U|\psi_a\rangle \hspace{1cm} \text{from equation (B.3)}$$

$$= \omega_a \sigma_z V^i|\psi_{a\oplus 1}\rangle \hspace{1cm} \text{from equation (5.5)}$$

$$= \omega_a \sigma_z|\psi_{a\oplus 1}(i)\rangle, \hspace{1cm} (B.4)$$

where we denote the sum modulo two by $\oplus$. Therefore, using the condition $\text{Tr} W^i = 0$ and the completeness relation with respect to $\{|\psi_a(i)\rangle\}_{a=1,2}$, we observe that

$$\gamma_a^\ast(k + 1 - i) = -\langle \psi_a(k-i) | W^{k+1-i} | \psi_a(k-i) \rangle$$

$$= -\langle \psi_{a\oplus 1}(i) | \sigma_z W^i \sigma_z | \psi_{a\oplus 1}(i) \rangle \hspace{1cm} \text{from equation (B.4) and } |\omega_a|^2 = 1$$

$$= (\psi_{a\oplus 1}(i)| W^i | \psi_{a\oplus 1}(i)) \hspace{1cm} \text{from equation (B.1)}$$

$$= \text{Tr}[W^i (1_2 - |\psi_a(i)\rangle\langle \psi_a(i)|)]$$

$$= -\langle \psi_a(i)| W^i | \psi_a(i) \rangle \hspace{1cm} \text{from Tr } W^i = 0$$

$$= -\langle \psi_a(i-1) | W^i | \psi_a(i-1) \rangle$$

$$= \gamma_a^\ast(i), \hspace{1cm} (B.5)$$

which proves equation (5.7).
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