Composite pulses in NMR as non-adiabatic geometric quantum gates

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We show that some composite pulses widely employed in nuclear magnetic resonance experiments are regarded as non-adiabatic geometric quantum gates with Aharonov-Andadan phases. Thus, we reveal the presence of a fundamental issue on quantum mechanics behind a traditional technique. To examine the robustness of such composite pulses against fluctuations, we present a simple noise model in a two-level system. Then, we find that the composite pulses possess purely geometrical nature even under a certain type of fluctuations.

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Geometric phases have been attracting a lot of attention from the view point of the foundation of quantum mechanics and mathematical physics [1, 2, 3, 4]. Recently, their application to quantum information processing is spotlighted [5, 6], because they are expected to be robust against noise. However, the robustness of a geometric quantum gate (GQG), which is a quantum gate only using geometric phases, is not completely verified. Various examinations on this issue have been reported [7, 8, 9, 10, 11, 12]. Biais and Tremblay [7] claimed that no advantage of the GQGs exists compared to the corresponding quantum gates with dynamical phases, while Zhu and Zanardi [8] showed that their non-adiabatic GQGs are robust against fluctuations in control parameters.

In this paper, we show that some composite pulses widely employed in nuclear magnetic resonance (NMR) [13, 14] to accomplish reliable operations is regarded as non-adiabatic GQGs based on an Aharonov-Andadan (AA) phase [15], and propose a simple noise model in a two-level system. Then, we classify fluctuations in terms of the robustness of the GQGs.

An AA phase appears under non-adiabatic cyclic time evolution of a quantum system [15]. We note that the generalization of the non-cyclic case is given in Ref. [6, 16]. Let us write the Bloch vector at $t$ ($0 \leq t \leq 1$) as $\mathbf{n}(t) \in \mathbb{R}^3$. We denote a state vector given $\mathbf{n}(t)$ as $|\mathbf{n}(t)\rangle \in \mathbb{C}^2$. Namely, $\mathbf{n}(t) = |\mathbf{n}(t)\rangle \sigma |\mathbf{n}(t)\rangle$, where $\sigma = \{\sigma_x, \sigma_y, \sigma_z\}$. The symbol $\sigma$ means the transposition of a vector. Time evolution is described by the Schrödinger equation with the Hamiltonian $H(t)$. Note that $|\mathbf{n}(t)\rangle = 1$. Hereafter, we denote $\mathbf{n}(0)$ as $\mathbf{n}$. We take the natural unit system in which $\hbar = 1$. Suppose that $|\mathbf{n}(1)\rangle = e^{\gamma t} |\mathbf{n}\rangle$ ($\gamma \in \mathbb{R}$); $\mathbf{n}(1) = \mathbf{n}$. The AA phase $\gamma_g$ is defined as [15]

$$\gamma_g = \gamma - \gamma_d, \tag{1}$$

where

$$\gamma_d = -\int_0^1 \langle \mathbf{n}(t)|H(t)|\mathbf{n}(t)\rangle dt \tag{2}$$

is a dynamical phase.

Next, suppose $\mathbf{n}_+$ and $\mathbf{n}_-$ are two Bloch vectors satisfying (a) $\mathbf{n}_+ \cdot \mathbf{n}_- = -1$ (i.e., $\langle \mathbf{n}_+ | \mathbf{n}_- \rangle = 0$) and (b) $\mathbf{n}_\pm(1) = \mathbf{n}_\pm$ (i.e., there exist $\gamma_\pm \in \mathbb{R}$ such that $|\mathbf{n}_\pm(1)\rangle = e^{\gamma_\pm t} |\mathbf{n}_\pm\rangle$). An arbitrary quantum state $|\mathbf{n}\rangle$ is expressed by $|\mathbf{n}\rangle = a_+ |\mathbf{n}_+\rangle + a_- e^{i\gamma_-} |\mathbf{n}_-\rangle$, where $a_+ = \langle \mathbf{n}_+ | \mathbf{n}\rangle$. We call $\mathbf{n}_\pm$ basis Bloch vector corresponding to $H(t)$. The initial state $|\mathbf{n}\rangle$ is transformed into the final state $|\mathbf{n}(1)\rangle = a_+ e^{i\gamma_+} |\mathbf{n}_+\rangle + a_- e^{i\gamma_-} |\mathbf{n}_-\rangle$. Thus, the time evolution operator $U(t)$ at $t = 1$ generated by $H(t)$ ($t \in [0, 1]$) is rewritten as

$$U = e^{i\gamma_+} |\mathbf{n}_+\rangle \langle \mathbf{n}_+| + e^{i\gamma_-} |\mathbf{n}_-\rangle \langle \mathbf{n}_-| \tag{3}$$

Equation (3) becomes a quantum gate with a geometric phase, when the dynamical component of $\gamma_\pm$ is vanishing.

Let us focus on the Hamiltonian for a one-qubit system,

$$H(t) = \frac{1}{2} \omega(t) \mathbf{m}(t) \cdot \mathbf{\sigma} \quad (0 \leq t \leq 1), \tag{4}$$

which is inspired by a NMR Hamiltonian. In the case of NMR, $\omega(t)$ and $\mathbf{m}(t)$ are the amplitude of and the unit vector parallel to a magnetic field, respectively. The dynamical phase vanishes when $\mathbf{m}(t) \cdot \mathbf{n}(t) = 0$ [17]. We note that the integrand in Eq. (2) is rewritten as $\langle \mathbf{n}(t)|H(t)|\mathbf{n}(t)\rangle$ and $\langle \mathbf{n}(t)|H(t)|\mathbf{n}(t)\rangle = (\omega(t)/4) \text{tr}[(\mathbf{m}(t) \cdot \mathbf{\sigma}) |\mathbf{n}(t)\rangle \langle \mathbf{n}(t)| \mathbf{\sigma}] = (\omega(t)/2) \mathbf{m}(t) \cdot \mathbf{n}(t)$, where we use $\text{tr}[H(t)] = 0$ and $\text{tr}(\mathbf{\sigma}_x \mathbf{\sigma}_y) = 2i\gamma_j$. This condition has been widely used in the experiments on non-adiabatic GQGs [8].

A series of pulses, $90^\circ, 180^\circ, 90^\circ$ has been widely employed in the field of NMR for wide band decoupling [13, 14], where $\beta_k$ denotes a spin rotation by the angle $\beta$ in degree around $k$-axis. This is called composite pulse and corresponds to the unitary operator $e^{-i\beta_\sigma_z/4}e^{-i\beta_\sigma_y/2}e^{-i\beta_\sigma_z/4}$, which is equal to $e^{-i\pi \sigma_y/2}$. This is generated by the Hamiltonian

$$H(t) = \pi \mathbf{m}(t) \cdot \mathbf{\sigma} \quad (0 \leq t \leq 1), \tag{5}$$

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The fluctuations are given by Eq. (5), where $f_0 = g_0 = 0.1$ and $\xi = \eta = 5$.

where

$$m(t) = \begin{cases} t(1, 0, 0) & (0 \leq t \leq 1/4) \\ t(1, 0, 0) & (1/4 \leq t \leq 3/4) \\ t(1, 0, 0) & (3/4 \leq t \leq 1) \end{cases}.$$ 

Hereafter, we will denote $t_0 = 0$, $t_1 = 1/4$, $t_2 = 3/4$, and $t_3 = 1$. Various types of composite pulses have been proposed [13, 14], and their usages have been also discussed in the context of NMR quantum computing [18].

Let us examine the time evolution generated by Hamiltonian (3) from the viewpoint of non-adiabatic GQGs. We choose $n_+ = e^{i(0, 0, 1)}$, where $n_+ \cdot n_- = -1$. Then, we have the explicit formula

$$n_\pm(t) = \pm \left( \sin \theta(t) \sin \phi(t), -\sin \theta(t) \cos \phi(t), \cos \theta(t) \right),$$

where

$$\theta(t) = 2\pi t - \frac{\pi}{2}, \quad \phi(t) = \begin{cases} \pi/2 & (t_1 \leq t \leq t_2) \\ 0 & \text{(otherwise)} \end{cases}.$$ 

The temporal behavior of $n_+$ on the Bloch sphere is shown in Fig. 1(a). The trajectory $n_+$ is closed. It means that $|n_+(1)\rangle = e^{i\gamma_+} |n_+(1)\rangle$. We find that $|n_+(1)\rangle = e^{\mp i\pi/2} |n_-\rangle$ via solving the Schrödinger equation. We note that $\gamma$ is a solid angle surrounded by the trajectory $n_+(t)$. We also find that $m(t) \cdot n_\pm(t) = 0$ at any $t \in [0, 1]$, and thus the dynamical component is vanishing. Accordingly, we obtain the non-adiabatic GQG, $U = e^{-i\pi/2} |n_+(1)\rangle \langle n_+| + e^{i\pi/2} |n_-\rangle \langle n_-| = e^{-i\pi\sigma_\phi/2}$. One of the most commonly employed composite pulses turns out a non-adiabatic GQG [19].

We will classify fluctuations in terms of robustness of the composite pulse $90_\circ 180_\circ 90_\circ$. A noise model will be proposed based on a fluctuated closed curve on the Bloch sphere. We examine the situation in which the radio-frequency (rf) amplitude and phase, and the resonance off-set are temporary fluctuated around their aimed values. The fluctuated curve is given by

$$\hat{n}_\pm(t) = \pm \left( \sin(\theta(t) + f(t)) \sin(\phi(t) + g(t)), -\sin(\theta(t) + f(t)) \cos(\phi(t) + g(t)), \cos(\theta(t) + f(t)) \right),$$

where we assume that $f(t)$ and $g(t)$ are continuous and smooth in $[0, 1]$ [20] and satisfy

$$f(t_0) = g(t_0) = 0, \quad f(t_3) = g(t_3) = 0.$$ 

We will discuss the relevance of $f(t)$ and $g(t)$ to fluctuations below. The trajectory $\hat{n}_+(t)$ is closed under the assumption (8), as shown in Fig. 1(b). Thus, we have

$$|\hat{n}_+(1)\rangle = e^{i\tilde{\gamma}_\pm} |\hat{n}_+\rangle,$$

with a phase $\tilde{\gamma}_\pm$. Generally, $\tilde{\gamma}_\pm$ includes both the dynamical and the geometric components. We employ this noise model in order to ensure the existence of a definite AA phase, although we aware of its artificiality. An analysis based on a non-cyclic geometric phase [12, 10] may be needed for more comprehensive discussions.

We derive the Hamiltonian generating the time evolution corresponding to Eq. (7). By differentiating Eq. (7) with respect to $t \in (t_{i-1}, t_i)$ ($i = 1, 2, 3$), we obtain the Bloch equation. Then, we find the Hamiltonian in this time interval. Hence, the Hamiltonian at $t \in [0, 1]$ is given by

$$\tilde{H}(t) = \frac{1}{2} \tilde{\omega}(t) \tilde{m}(t) \cdot \sigma + \frac{1}{2} \frac{dg(t)}{dt} \sigma_z,$$

where

$$\tilde{\omega}(t) = 2\pi + \frac{df(t)}{dt}, \quad \tilde{m}(t) = \begin{pmatrix} \cos(\phi(t) + g(t)) \\ \sin(\phi(t) + g(t)) \end{pmatrix}.$$ 

We find that

$$\tilde{m}(t) \cdot \tilde{n}(t) = 0.$$ 

at any $t \in [0, 1]$. The derivative of $f(t)$ is a fluctuation of the rf amplitude, while that of $g(t)$ is that of the resonance off-set. A fluctuation of the rf phase is described by $g(t)$. From Eq. (2), the dynamical component $\gamma_{d\pm}$ of $\tilde{\gamma}_\pm$ is given by

$$\gamma_{d\pm} = \pm \frac{1}{2} \int_{t_0}^{t_3} \frac{dg(t)}{dt} \cos(\theta(t) + f(t)) \ dt.$$ 

We show that the following two cases exactly lead to $\gamma_{d\pm} = 0$. Namely, (i) $g(t) = 0$ and (ii) $f(t)$ and $g(t)$ have a certain symmetric property under time translation. The validity of the case (i) is obvious from Eq. (12). We focus on the case (ii). We note that $90_\circ 180_\circ 90_\circ$ has several interesting properties under time translation: $\theta(t + 1/2) = \theta(t) + \pi$. For example, we divide the total time interval $I_{all} = \{ t \in [t_0, t_3] \}$ into the four intervals, $I_1 = \{ t \in [t_0, t_1] \}, I_2 = \{ t \in [t_1, 1/2] \}, I_3 = \{ t \in [1/2, t_2] \}, I_4 = \{ t \in [t_2, t_3] \}$.
settling a desired strength. One can also encounter the
It is necessary to examine the case (iii) by numerically solving the Schrödinger equation
with Eq. (10). The case (i) often happens in experiments.

\begin{align*}
I_3 = \{ t \in [1/2, t_2] \}, \quad &I_4 = \{ t \in [t_2, t_3] \}. \text{ Let us consider a case when the conditions} \\
&f(t + 1/2) = f(t), \quad \frac{df}{dt}(t + 1/2) = \frac{df}{dt}(t), \quad (13)
\end{align*}

are satisfied. The contribution from \(I_1 \) (\(I_2\)) is canceled out by that from \(I_3 \) (\(I_4\)). Thus, this case leads to \(\tilde{\gamma}_{d+} = 0\). Let us consider another case, in which the conditions

\begin{align*}
f(1-t) = -f(t), \quad \frac{df}{dt}(1-t) = \frac{df}{dt}(t), \quad (14)
\end{align*}

are satisfied. We note that \(f(1/2) = 0\) is imposed in Eq. (14). In this case, the contribution from \(I_1 \) (\(I_2\)) is canceled out by \(I_4 \) (\(I_3\)). This cancellation is related to the symmetry \(\theta(1-t) = -\theta(t) + \pi\). When \(f(t)\) and \(g(t)\) have a certain symmetric property compatible with the pulse sequence, the dynamical phase is vanishing. In addition, a case (iii) \(f(t)\) and \(g(t)\) rapidly oscillate with no correlation, leads to \(\tilde{\gamma}_{d+} \approx 0\). We can confirm the validity of the case (iii) by numerically solving the Schrödinger equation with Eq. (10). The case (i) often happens in experiments. From Eq. (10), one can find \(f(t)\) is associated only with the amplitude of an external control field. This quantity often shows an overshoot or an undershoot before settling a desired strength. One can also encounter the case (ii) in experiments. A typical example for Eq. (10) may be an oscillating function, as shown in Eq. (10). A linear combination of such oscillating functions leads to \(\tilde{\gamma}_{d+} = 0\). Thus, we expect that a lot of rapid oscillating fluctuations approximately satisfy Eqs. (13) or (14), and then \(\tilde{\gamma}_{d+} \approx 0\). The case (iii) is natural when the origins of \(f(t)\) and \(g(t)\) are independent. These three conditions lead to \(\tilde{\gamma}_{d+} = 0\). Thus, the quantum gate under them is still regarded as a GQG. It is necessary to examine about more realistic control processes [21, 22]. Nevertheless, the present discussion is meaningful to understand nature of robustness of a geometric phase.

We directly solve the Schrödinger equation with Eq. (10) in order to calculate the geometric component of \(\tilde{\gamma}_{d+}\). First, we choose

\begin{align*}
f(t) = f_0 \sin[2\pi \xi u_i(t)], \quad &g(t) = g_0 \sin[2\pi \eta u_i(t)], \quad (15)
\end{align*}

at \(t \in [t_{i-1}, t_i]\), where \(u_i(t) = (t - t_{i-1})/(t_i - t_{i-1})\) and \(\xi, \eta \in N\). The above functions are piecewise smooth in \([t_0, t_3]\) [20]. We show that the temporal evolution of the basis Bloch vector \(\hat{\mathbf{r}}(0, 1, 0)\) during the composite pulse 90°, 180°, 90° \(x\) with the fluctuations in Fig. 1(b). This example corresponds to the case (ii), since Eq. (14) is satisfied. We display the temporal behaviors of \(|\mathbf{n}_+(t)\rangle\) and \(|\mathbf{\hat{n}}_+(t)\rangle\) in Fig. 2. The state vector \(|\mathbf{\hat{n}}_+(t)\rangle\) is fluctuated around \(|\mathbf{n}_+(t)\rangle\), but \(|\mathbf{n}_+(t)\rangle\) is not. We find that \(\tilde{\gamma}_d = \mp \pi/2\). Thus, \(\tilde{\gamma}_{d+} = \mp \pi/2\) is confirmed. Let us discuss another example,

\begin{align*}
f(t) = f_0 \sin(8\pi \xi t), \quad &g(t) = g_0 \sin(8\pi \eta t), \quad (16)
\end{align*}

where \(f_0 \) (\(g_0\)) is a positive real number and \(\xi \) (\(\eta\)) is an integer \((t_0 \leq t \leq t_3)\). The above functions also satisfy Eq. (8). Solving the Schrödinger equation numerically leads to \(\tilde{\gamma}_{d+} = \mp \pi/2\). The above results mean that the solid angle surrounded by \(\mathbf{n}_+\) is always \(\pi\). We conjecture that, as long as the fluctuations are introduced by Eqs. (7) and (8), no dynamical phase should exactly lead \(\tilde{\gamma}_{d+} \neq \gamma_{d+}\).

It is interesting to study the case in which \(\mathbf{m}(t) \cdot \mathbf{n}(t) \neq 0\). Let us consider a simple operation on the Bloch sphere: \(\hat{\mathbf{H}}_A = \hat{\mathbf{H}}_B = \pi/4\) and \(H_B = \pi(\sigma_x + \sigma_y)/2\sqrt{2}\). The former satisfies the condition \(\mathbf{m}(t) \cdot \mathbf{n}(t) = 0\), but the latter does not. We describe fluctuations in the two models such as Eq. (10),

\begin{align*}
\hat{\mathbf{H}}_A(t) = (\frac{\pi}{2} + \frac{df}{dt}) \hat{\mathbf{m}}_A(t) \cdot \hat{\mathbf{\sigma}} + \frac{dg_0}{dt} \hat{\mathbf{\sigma}}_z, \\
\hat{\mathbf{H}}_B(t) = (\frac{\pi}{2} + \frac{df}{dt}) \hat{\mathbf{m}}_B(t) \cdot \hat{\mathbf{\sigma}} + \frac{dg_0}{dt} \hat{\mathbf{\sigma}}_z,
\end{align*}

where \(\hat{\mathbf{m}}_A(t) = \hat{\mathbf{m}}_B(t) = \hat{\mathbf{H}}_A(t) \hat{\mathbf{H}}_B(t)\) maps \(\gamma(0, 0, 1) \rightarrow \gamma(1, 0, 0)\) even in the presence of \(f(t)\) and \(g(t)\). On the other hand, the numerical calculation reveals that the one generated by \(\hat{\mathbf{H}}_A(t)\) maps \(\gamma(0, 0, 1) \rightarrow \gamma(0.95, -0.26, -0.16)\) [Fig. 3]. The results mean that Eq. (8) does not always ensure robustness in the present model. We can find an additional term appears in Eq. (0) when \(\mathbf{m}(t) \cdot \mathbf{n}(t) \neq 0\). Thus, it may cause a strong fluctuation. We guess that \(\mathbf{m}(t) \cdot \mathbf{n}(t) = 0\) might play an important role for stable time evolution in the present model.
In conclusion, we showed that the composite pulse 90°, 180°, 90° is regarded as a non-adiabatic GQG. In addition, we proposed a simple noise model based on a fluctuated curve on the Bloch sphere, and then classified fluctuations in terms of robustness of 90°, 180°, 90°. Although the present analysis is artificial, it is suitable for evaluating errors in non-adiabatic GQGs since a definite geometric phase exists even in the presence of fluctuations. It is important to improve the present method in order to examine a more realistic control process or a stochastic process. The fluctuations that we discussed should be called regular fluctuations, because the fluctuations are expressed by the two smooth functions f(t) and g(t). On the other hand, when fluctuations are given by uniform random variables, even a cyclic evolution may not be guaranteed and thus the robustness is not expected as discussed in Ref. [7]. We emphasize that it is important to specify fluctuations in order to evaluate robustness of a gate.

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