

Composite pulses in NMR as nonadiabatic geometric quantum gates

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We show that some composite pulses widely employed in NMR experiments are regarded as nonadiabatic geometric quantum gates with Aharonov-Anandan 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 possesses 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 [1–4]. 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 [7–12]. Blais 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 nonadiabatic GQGs are robust against fluctuations in control parameters.

In this Brief Report, we show that some composite pulses widely employed in nuclear magnetic resonance (NMR) [13,14] to accomplish reliable operations is regarded as nonadiabatic GQGs based on an Aharonov-Anandan (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 nonadiabatic cyclic time evolution of a quantum system [15]. We note that the generalization to the noncyclic case is given in Ref. [3,16]. 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, $\mathbf{n}(t) = \langle \mathbf{n}(t) | \boldsymbol{\sigma} | \mathbf{n}(t) \rangle$, where $\boldsymbol{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$. The symbol t means the transposition of a vector. Time evolution is described by the Schrödinger equation with the Hamiltonian $H(t)$. Note that $|\mathbf{n}(t)| = 1$. Hereafter, we denote $\mathbf{n}(0)$ as \mathbf{n} . We take the natural unit system in which $\hbar = 1$. Suppose that $|\mathbf{n}(1)\rangle = e^{i\gamma} |\mathbf{n}\rangle$ ($\gamma \in \mathbb{R}$): $\mathbf{n}(1) = \mathbf{n}$. The AA phase γ_g is defined as [15]

$$\gamma_g = \gamma - \gamma_d, \quad (1)$$

where

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

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 $|\mathbf{n}_\pm(1)\rangle = e^{i\gamma_\pm} |\mathbf{n}_\pm\rangle$). An arbitrary quantum state $|\mathbf{n}\rangle$ is expressed by $|\mathbf{n}\rangle = a_+ |\mathbf{n}_+\rangle + a_- |\mathbf{n}_-\rangle$, where $a_\pm = \langle \mathbf{n}_\pm | \mathbf{n} \rangle$. 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 at $t=1$ generated by $H(t)$ ($t \in [0, 1]$) is rewritten as

$$U = e^{i\gamma_+} |\mathbf{n}_+\rangle \langle \mathbf{n}_+| + e^{i\gamma_-} |\mathbf{n}_-\rangle \langle \mathbf{n}_-|. \quad (3)$$

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

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

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

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 $\langle \mathbf{n}(t) | H(t) | \mathbf{n}(t) \rangle = (\omega(t)/4) \text{tr}[(\mathbf{m}(t) \cdot \boldsymbol{\sigma})(\mathbf{n}(t) \cdot \boldsymbol{\sigma})] = (\omega(t)/2) \mathbf{m}(t) \cdot \mathbf{n}(t)$, where we use $\text{tr}[H(t)] = 0$ and $\text{tr}(\sigma_i \sigma_j) = 2\delta_{ij}$. This condition has been widely used in the experiments on nonadiabatic GQGs [6].

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

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

where

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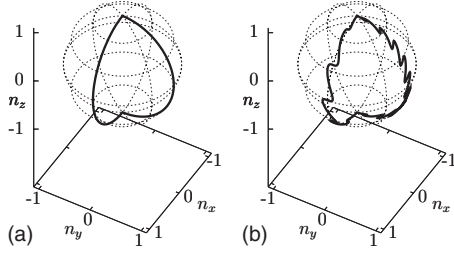


FIG. 1. Temporal behavior of the basis Bloch vector ${}^t(0,1,0)$ during the composite pulse $90_x 180_y 90_x$. (a) without and (b) with fluctuations in the control parameters. The fluctuations are given by Eq. (15), where $f_0=g_0=0.1$ and $\xi=\eta=5$.

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

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 (5) from the view point of nonadiabatic GQGs. We choose $\mathbf{n}_\pm = {}^t(0, \pm 1, 0)$, where $\mathbf{n}_+ \cdot \mathbf{n}_- = -1$. Then, we have the explicit formula

$$\mathbf{n}_\pm(t) = \pm \begin{pmatrix} \sin \theta(t) \sin \phi(t) \\ -\sin \theta(t) \cos \phi(t) \\ \cos \theta(t) \end{pmatrix}, \quad (6)$$

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

We will classify fluctuations in terms of robustness of the composite pulse $90_x 180_y 90_x$. 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

$$\tilde{\mathbf{n}}_\pm(t) = \pm \begin{pmatrix} \sin[\theta(t) + f(t)] \sin[\phi(t) + g(t)] \\ -\sin[\theta(t) + f(t)] \cos[\phi(t) + g(t)] \\ \cos[\theta(t) + f(t)] \end{pmatrix}, \quad (7)$$

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

$$f(t_0) = g(t_0) = 0, \quad f(t_3) = g(t_3) = 0. \quad (8)$$

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

$$|\tilde{\mathbf{n}}_\pm(1)\rangle = e^{i\tilde{\gamma}_\pm}|\tilde{\mathbf{n}}_\pm\rangle, \quad (9)$$

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 noncyclic geometric phase [12,16] 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

$$\tilde{H}(t) = \frac{1}{2} \tilde{\omega}(t) \tilde{\mathbf{m}}(t) \cdot \boldsymbol{\sigma} + \frac{1}{2} \frac{dg(t)}{dt} \sigma_z, \quad (10)$$

where

$$\tilde{\omega}(t) = 2\pi + \frac{df(t)}{dt}, \quad \tilde{\mathbf{m}}(t) = \begin{pmatrix} \cos[\phi(t) + g(t)] \\ \sin[\phi(t) + g(t)] \\ 0 \end{pmatrix}.$$

We find that

$$\tilde{\mathbf{m}}(t) \cdot \tilde{\mathbf{n}}(t) = 0. \quad (11)$$

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 $\tilde{\gamma}_{d\pm}$ of $\tilde{\gamma}_\pm$ is given by

$$\tilde{\gamma}_{d\pm} = \mp \frac{1}{2} \int_{t_0}^{t_3} \frac{dg(t)}{dt} \cos[\theta(t) + f(t)] dt. \quad (12)$$

We show that the following two cases exactly lead to $\tilde{\gamma}_{d\pm} = 0$. 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 $90_x 180_y 90_x$ has several interesting properties under time translation: $\theta(t+1/2) = \theta(t) + \pi$, for example. We divide the total time interval $I_{\text{all}} = \{t \in [t_0, t_3]\}$ into the four intervals, $I_1 = \{t \in [t_0, t_1]\}$, $I_2 = \{t \in [t_1, 1/2]\}$, $I_3 = \{t \in [1/2, t_2]\}$, and $I_4 = \{t \in [t_2, t_3]\}$. Let us consider a case when the conditions

$$f(t+1/2) = f(t), \quad \frac{dg}{dt}(t+1/2) = \frac{dg}{dt}(t), \quad (13)$$

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

$$f(1-t) = -f(t), \quad \frac{dg}{dt}(1-t) = \frac{dg}{dt}(t), \quad (14)$$

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

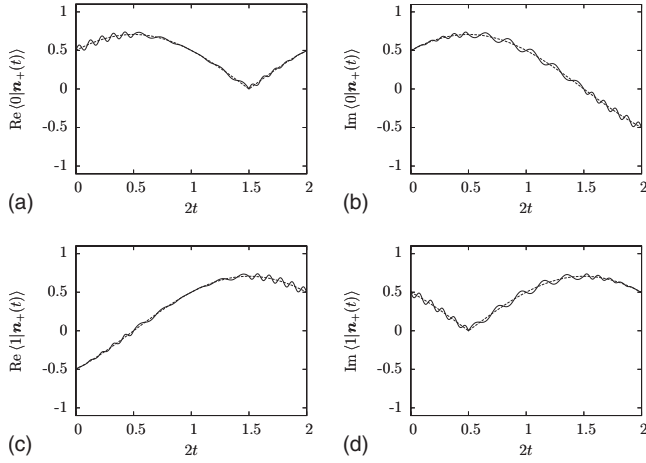


FIG. 2. Temporal behavior of the state vector corresponding to the basis Bloch vector ${}^t(0, 1, 0)$ during $90_x 180_y 90_x$. The initial state vectors are chosen as $|\mathbf{n}_+\rangle = e^{i\pi/4}(|0\rangle + i|1\rangle)/\sqrt{2}$. The solid line is the model with the fluctuations. The fluctuations are described by Eq. (15), where $f_0 = g_0 = 0.1$ and $\xi = \eta = 5$. The dashed line is the ideal case. (a) $\text{Re}\langle 0|\mathbf{n}_+(t)\rangle$. (b) $\text{Im}\langle 0|\mathbf{n}_+(t)\rangle$. (c) $\text{Re}\langle 1|\mathbf{n}_+(t)\rangle$. (d) $\text{Im}\langle 1|\mathbf{n}_+(t)\rangle$.

$I_4(I_3)$. 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 $\tilde{\gamma}_{d\pm} \approx 0$. 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 controlled 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. (13) may be an oscillating function, as shown in Eq. (16). A linear combination of such oscillating functions leads to $\tilde{\gamma}_{d\pm} = 0$. Thus, we expect that a lot of rapid oscillating fluctuations approximately satisfy Eqs. (13) and (14), and then $\tilde{\gamma}_{d\pm} \approx 0$. The case (iii) is natural when the origins of $f(t)$ and $g(t)$ are independent. These three conditions lead to $\tilde{\gamma}_{d\pm} = 0$. 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 $\tilde{\gamma}_{\pm}$. First, we choose

$$f(t) = f_0 \sin[2\pi\xi u_i(t)], \quad g(t) = g_0 \sin[2\pi\eta u_i(t)], \quad (15)$$

at $t \in [t_{i-1}, t_i]$, where $u_i(t) = (t - t_{i-1}) / (t_i - t_{i-1})$ and $\xi, \eta \in \mathbb{N}$. The above functions are piecewise smooth in $[t_0, t_3]$ [20]. We show that the temporal evolution of the basis Bloch vector ${}^t(0, 1, 0)$ during the composite pulse $90_x 180_y 90_x$ 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 $|\tilde{\mathbf{n}}_+(t)\rangle$ in Fig. 2. The state vector

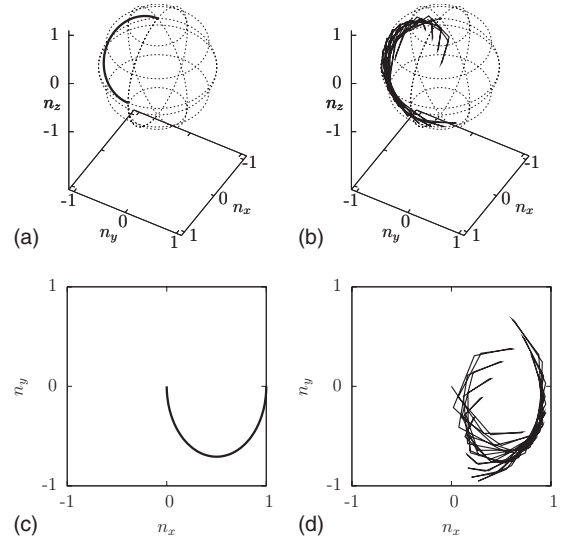


FIG. 3. Temporal behavior of the Bloch vector starting from ${}^t(0, 0, 1)$ under the Hamiltonian H_B is shown in (a) and its trajectory projected on $n_x n_y$ -plane is shown in (c). The final point is ${}^t(1, 0, 0)$. Temporal behavior of the Bloch vector starting from ${}^t(0, 0, 1)$ under the fluctuating Hamiltonian \tilde{H}_B ($f_0 = g_0 = 1.0$ and $\xi = \eta = 10$ in Eq. (16)) is shown in (b) and its trajectory projected on $n_x n_y$ plane is shown in (d). The final point is ${}^t(0.95, -0.26, -0.16)$.

$|\tilde{\mathbf{n}}_+(t)\rangle$ is fluctuated around $|\mathbf{n}_+(t)\rangle$, but $|\tilde{\mathbf{n}}_+(t_3)\rangle = |\mathbf{n}_+(t_3)\rangle$. We find that $\tilde{\gamma}_{\pm} = \mp \pi/2$. Thus, $\tilde{\gamma}_{g\pm} = \mp \pi/2$ is confirmed. Let us discuss another example,

$$f(t) = f_0 \sin(8\pi\xi t), \quad g(t) = g_0 \sin(8\pi\eta t), \quad (16)$$

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 $\tilde{\gamma}_{\pm} = \tilde{\gamma}_{g\pm} = \mp \pi/2$. The above results mean that the solid angle surrounded by $\tilde{\mathbf{n}}_{\pm}(t)$ is always π . We conjecture that, as long as the fluctuations are introduced by Eqs. (7) and (8), no dynamical phase should exactly lead to $\tilde{\gamma}_{g\pm} = \gamma_{g\pm}$.

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: ${}^t(0, 0, 1) \rightarrow {}^t(1, 0, 0)$. This process is realized by using either $e^{-iH_A t}$ or $e^{-iH_B t}$ ($0 \leq t \leq 1$), where $H_A = \pi\sigma_y/4$ and $H_B = \pi(\sigma_x + \sigma_z)/2\sqrt{2}$. 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),

$$\tilde{H}_A(t) = \left(\frac{\pi}{2} + \frac{df}{dt} \right) \frac{\tilde{\mathbf{m}}_A(t) \cdot \boldsymbol{\sigma}}{2} + \frac{dg}{dt} \frac{\sigma_z}{2},$$

$$\tilde{H}_B(t) = \left(\frac{\pi}{\sqrt{2}} + \frac{df}{dt} \right) \frac{\tilde{\mathbf{m}}_B(t) \cdot \boldsymbol{\sigma}}{2} + \left(\frac{\pi}{\sqrt{2}} + \frac{dg}{dt} \right) \frac{\sigma_z}{2},$$

where $\tilde{\mathbf{m}}_A(t) = {}^t(\cos[\pi/2 + g(t)], \sin[\pi/2 + g(t)], 0)$ and $\tilde{\mathbf{m}}_B(t) = {}^t(\cos g(t), \sin g(t), 0)$. Since $f(0) = f(1) = g(0) = g(1) = 0$, which corresponds to Eq. (8), the unitary operator generated by $\tilde{H}_A(t)$ maps ${}^t(0, 0, 1) \rightarrow {}^t(1, 0, 0)$ even in the presence of $f(t)$ and $g(t)$. On the other hand, the numerical calculation reveals that the one generated by $\tilde{H}_B(t)$ maps

${}^t(0, 0, 1) \rightarrow {}^t(0.95, -0.26, -0.16)$ [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. (6) when $\mathbf{m}(t) \cdot \mathbf{n}(t) \neq 0$. Thus, it may cause a large error in operation. We guess that $\mathbf{m}(t) \cdot \mathbf{n}(t) = 0$ plays an important role for stable time evolution in the present model.

In conclusion, we showed that the composite pulse $90_x 180_y 90_x$ is regarded as a nonadiabatic 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 $90_x 180_y 90_x$. Although the present analysis is artificial, it is suitable for evaluating errors in nonadiabatic 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 realis-

tic 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 [23] 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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