

Validity of the rotating-wave approximation in nonadiabatic holonomic quantum computation

Jakob Spiegelberg¹ and Erik Sjöqvist^{1,2}

¹*Department of Quantum Chemistry, Uppsala University, Box 518, SE-751 20 Uppsala, Sweden*

²*Centre for Quantum Technologies, National University of Singapore, 3 Science Drive 2, 117543 Singapore, Singapore*

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We examine the validity of the rotating-wave approximation (RWA) in nonadiabatic holonomic single-qubit gates [New J. Phys. **14**, 103035 (2012)]. We demonstrate that the adoption of RWA may lead to a sharp decline in fidelity for rapid gate implementation and small energy separation between the excited and computational states. The validity of the RWA in the recent experimental realization [Nature (London) **496**, 482 (2013)] of nonadiabatic holonomic quantum computation for a superconducting qubit is examined.

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Holonomic quantum computation (HQC) is the idea of using non-Abelian geometric phases to implement robust quantum gates [1]. By using adiabatic holonomies, HQC becomes tolerant to errors caused by fluctuations of the slowly changing control parameters. On the other hand, dissipation may have detrimental effects on the gates, leading to the need to perform the gate operations as fast as possible by using nonadiabatic holonomies. Nonadiabatic strategies have been shown [2] to be effective to minimize this error source. However, a shortening of the run time may in turn lead to other errors that can lower the gate fidelity and therefore put a limitation on the speed of holonomic gate operations. Here, we examine how the validity of the rotating-wave approximation (RWA) depends on the run time and energy structure of the three-level Λ setting used to implement nonadiabatic non-Abelian geometric gates first proposed in Ref. [3] and experimentally demonstrated in Refs. [4,5].

The speed of quantum gate operations is generally limited by unwanted effects that become more pronounced when the run time is decreased. One such effect is related to the quasimonochromatic approximation [6] that breaks down for short pulses, causing population of energy levels outside the computational subspace [7,8]. Another speed-limiting feature is the RWA, which is expected to break down when the run time of the gate becomes too short. This leads to a situation where the Rabi flopping is accompanied by faster fidelity-reducing oscillations [9], an effect that can be suppressed by embedding the qubit in an off-resonant Λ system [10]. We quantify the validity of the RWA by computing the fidelity of the ideal RWA-based nonadiabatic holonomic single-qubit gate operations with respect to numerical solutions of the exact Schrödinger equation.

The Λ system consists of states $|0\rangle$ and $|1\rangle$ coupled to the auxiliary excited state $|e\rangle$ via a pair of oscillating electric field pulses $\mathbf{E}_j(t) = \epsilon_j g_j(t) \cos(\omega_j t)$, $j = 0, 1$, $g_j(t)$ being envelope functions describing the pulse shape and duration. The polarization $\epsilon_j(t)$ is chosen so as to allow for the $j \leftrightarrow e$ transition only. The Hamiltonian of the system reads $\hat{H}(t) = \hat{H}_0 + \hat{\boldsymbol{\mu}} \cdot [\mathbf{E}_0(t) + \mathbf{E}_1(t)]$, where $\hat{H}_0 = -f_{e0} |0\rangle \langle 0| - f_{e1} |1\rangle \langle 1|$ is the bare Hamiltonian (by putting the energy of the excited state to zero) and $\hat{\boldsymbol{\mu}}$ is the electric dipole operator. By tuning the oscillation frequencies ω_j on resonance with the bare transition frequencies f_{ej} , the Hamiltonian in the

interaction picture reads

$$\hat{H}_I(t) = \Omega_0(t)(1 + e^{-2if_{e0}t}) |e\rangle \langle 0| + \Omega_1(t)(1 + e^{-2if_{e1}t}) |e\rangle \langle 1| + \text{H.c.}, \quad (1)$$

where $\Omega_j(t) = \langle e | \hat{\boldsymbol{\mu}} \cdot \boldsymbol{\epsilon}_j | j \rangle g_j(t) / (2\hbar)$. The RWA means that the $e^{\pm 2if_{ej}t}$ terms oscillate rapidly enough so that they can be neglected in $\hat{H}_I(t)$.

Provided the RWA applies, a nonadiabatic holonomic gate $\hat{U}(C)$ acting on the computational subspace spanned by $|0\rangle$ and $|1\rangle$ is implemented by choosing electric field pulses such that $\Omega_0(t)/\Omega_1(t)$ is time independent and the π pulse criterion $\int_0^\tau \sqrt{|\Omega_0(t)|^2 + |\Omega_1(t)|^2} dt = \pi$ is satisfied. Here, the latter condition assures that the computational subspace undergoes a cyclic evolution around the path C in the Grassmannian $G(3; 2)$ [11]; the former guarantees that the dynamical phases vanish for the full pulse duration, which implies that the gate is fully determined by C [3]. Explicitly,

$$\hat{U}(C) = \sin \theta \cos \phi \hat{\sigma}_x + \sin \theta \sin \phi \hat{\sigma}_y + \cos \theta \hat{\sigma}_z, \quad (2)$$

where $\Omega_0(t)/\Omega_1(t) = -\tan(\theta/2)e^{i\phi}$ and $\hat{\sigma}_k$, $k = x, y, z$ are the standard Pauli operators acting on the computational subspace. Here, we examine the gate fidelity by comparing the ideal holonomic RWA-based transformation $|\psi\rangle \mapsto \hat{U}(C)|\psi\rangle$ with the transformation $|\psi\rangle \mapsto \mathbf{T}e^{-(i/\hbar)\int_0^\tau \hat{H}_I(t)dt} |\psi\rangle$ obtained by numerically solving the exact Schrödinger equation for $\hat{H}_I(t)$, in order to determine the range of validity of the RWA. The gate fidelity for an input state $|\psi\rangle$ is given by $|\langle \psi | U^\dagger(C) \mathbf{T}e^{-(i/\hbar)\int_0^\tau \hat{H}_I(t)dt} |\psi \rangle|$, i.e., the overlap between the exact and the ideal RWA-based outputs. \mathbf{T} denotes time ordering.

In order to test the validity of the RWA, the dependence of the fidelity on transition frequencies, pulse shape, and pulse duration is examined. As holonomic test gates, we choose the NOT gate $|x\rangle \mapsto |x \oplus 1\rangle$, where $x = 0, 1$ and \oplus is addition modulo 2, which is achieved in the RWA regime by setting $\Omega_0(t)/\Omega_1(t) = 1$, and the Hadamard gate $|x\rangle \mapsto \frac{1}{\sqrt{2}}[(-1)^x |x\rangle + |x \oplus 1\rangle]$, where $\Omega_0(t)/\Omega_1(t) = -\tan(\frac{\pi}{8})$.

In Table I, fidelities for a range of transition frequencies $f \equiv f_{e0} = f_{e1}$ are displayed for the two gate operations acting on the input state $|0\rangle$. In both cases, three different regions can be identified: For large f_{ej} , the RWA is valid and the exact and ideal output states nearly coincide, leading to a fidelity

TABLE I. Fidelity of holonomic NOT and Hadamard gates for different transition frequencies $f \equiv f_{e0} = f_{e1}$. We use a truncated Gaussian-shaped pulse with full width at half maximum (FWHM) = 10 ns, a total duration of 40 ns, and input state $|0\rangle$.

f [s^{-1}]	NOT	Hadamard
10^6	0.0037	0.7071
10^7	0.0394	0.7004
10^8	0.8543	0.7903
5×10^8	0.9750	0.9712
10^9	0.9990	0.9994
10^{10}	1.0000	1.0000

close to unity. For small energy separations, the additional exponential term leads to a factor of 2 since $1 + e^{2if_{ej}t} \approx 2$. The quantum system runs the cyclic evolution twice. One property of the matrices representing Hadamard and NOT gate is that their product with themselves is the identity matrix; the new transformation resembles the identity operation that preserves the input state. In the case of the NOT gate, the overlap between the input state $|0\rangle$ and the output state after running through a NOT gate vanishes per definition. For the Hadamard gate, the overlap between input state $|0\rangle$ and Hadamard transformed state is $1/\sqrt{2} \approx 0.7071$. In the third region, between these extremes, the RWA leads to oscillations of the overlap. The impact on the system would be highly dependent upon the precise timing of the laser pulses and the corresponding operation would therefore not represent a simple quantum gate in this region. These findings still hold for a situation where the transition frequencies are not equal, i.e., $f_{e0} \neq f_{e1}$.

Next, five different pulse shapes are tested for the $+1$ eigenstates $|0\rangle$, $\frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$, $\frac{1}{\sqrt{2}}(|0\rangle + i|1\rangle)$ of the three Pauli operators $\hat{\sigma}_x, \hat{\sigma}_y, \hat{\sigma}_z$ as input. A truncated Gaussian pulse with the full width at half maximum (FWHM) as one fourth of the full pulse duration, a secant pulse, a parabolic pulse, a \sin^2 pulse, and a square pulse. The fidelities for the respective cases are enlisted in Table II. There are only small differences in the fidelity for different pulse shapes. However, the truncated Gaussian pulse leads to comparably low fidelities. An explanation for this deviation can be found in Table III. Since the FWHM of the truncated Gaussian pulse is chosen as one fourth of the absolute pulse duration, the region where the envelope is significantly different from zero is in the same order of magnitude as the FWHM. We suspect that only these regions contribute significantly to the system

TABLE II. Fidelity of holonomic NOT gate for different envelope functions and the $+1$ eigenstates of $\hat{\sigma}_x, \hat{\sigma}_y, \hat{\sigma}_z$, respectively, as input states. All other system parameters are taken from Ref. [4].

Envelope	$\frac{1}{\sqrt{2}}(0\rangle + 1\rangle)$	$\frac{1}{\sqrt{2}}(0\rangle + i 1\rangle)$	$ 0\rangle$
Truncated Gaussian	0.9999	0.9853	0.9861
sech	0.9956	0.9953	0.9947
Parabola	0.9991	0.9988	0.9988
\sin^2	0.9975	0.9962	0.9959
Square	0.9991	0.9989	0.9980

TABLE III. Fidelity of the input state $|0\rangle$ after a NOT transformation for a selection of total durations of the pulses. All other system parameters are taken from Ref. [4].

Envelope	100 ns	40 ns	10 ns	2.5 ns
Truncated Gaussian	0.9987	0.9861	0.8072	0.1790
sech	0.9995	0.9947	0.9792	0.6703
Parabola	0.9997	0.9988	0.9987	0.8573
\sin^2	0.9996	0.9959	0.9857	0.4424
Square	0.9998	0.9980	0.9991	0.7952

dynamics. Hence, the truncated Gaussian pulse for 40 ns is comparable to a 10-ns pulse of the other shapes.

Very short laser pulses have the advantage that dissipation can be neglected. However, the RWA leads to instabilities in the quantum gate, if the time scale becomes too short. The fidelity achieved with a truncated Gaussian laser pulse as a function of the total pulse duration is shown in Fig. 1. The calculation is based on averaging the output state overlap over the input states $|0\rangle$, $\frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$, $\frac{1}{\sqrt{2}}(|0\rangle + i|1\rangle)$. For both gates examined, the fidelity is stable over a wide range. Upon some threshold, the fidelity begins to fluctuate heavily and deteriorates quickly, in this case at approximately 20 ns.

Abdumalikov *et al.* [4] experimentally realized gate operations on a Λ system implemented in a transmon superconducting qubit, following the proposal in Ref. [3]. Their transition frequencies were $f_{e0} \approx 5.0806 \times 10^{10} s^{-1}$ and $f_{e1} \approx 4.8580 \times 10^{10} s^{-1}$; their truncated Gaussian shaped pulse had a FWHM of 10 ns and a full duration of 40 ns. This choice of parameters lies relatively close to the edge of the zone with stable fidelity. If a further speedup of the computation should be achieved, a larger separation of the energy levels has to be aimed for.

In holonomic quantum computing, noncommuting gates can be implemented. Here, we studied the influence of the RWA on the fidelity after application of the two possible combinations of NOT and Hadamard gate and compared these with the fidelity obtained by multiplying the fidelities for separate NOT and Hadamard gate, i.e., the fidelity as if the two

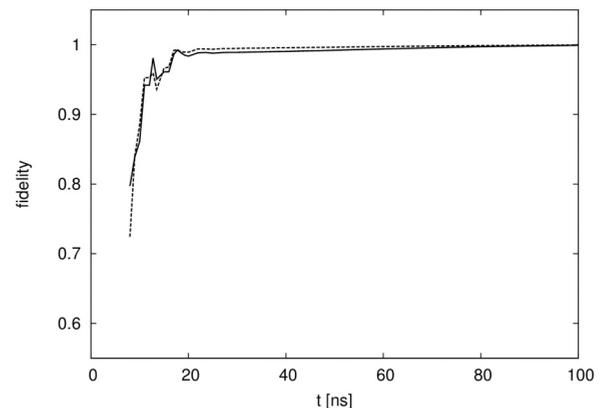


FIG. 1. Dependence of the fidelity on the pulse duration for the NOT gate (continuous line) and the Hadamard gate (dashed line). A truncated Gaussian pulse is used. All other system parameters are taken from Ref. [4].

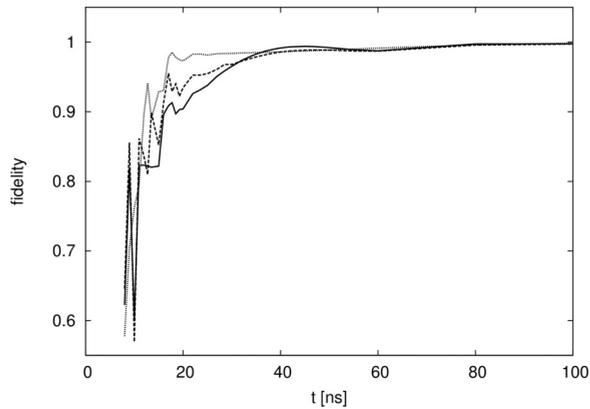


FIG. 2. Dependence of the fidelity on the pulse duration for the combinations of Hadamard and NOT gate (continuous line), NOT and Hadamard gate (dashed line), and the product of the fidelities of the NOT and Hadamard gates separately (dotted line). The duration plotted here equals the duration of each of the pulses and thereby half of the combined gate's duration. A truncated Gaussian pulse is used. All other system parameters are taken from Ref. [4].

gates were commuting. In our model, the two pulses followed each other without any separation in time.

As can be seen in Fig. 2, the fidelity achieved with the noncommuting gates is typically lower than the product of their fidelities. Furthermore, the fidelity decreases at pulse durations around 40 ns. This decline appears earlier than expected, taking the multiplied gate fidelities of the separate gates as reference. We conclude that this effect occurs due to the non-Abelian nature of the gates. The fluctuations, which were previously only significant in the short duration regime, are now visible throughout the entire range of durations studied. The noncommutativity of Hadamard and NOT gate can be clearly seen by comparison of the H-NOT and NOT-H combinations in Fig. 2.

To conclude, the rotating-wave approximation (RWA) has been proven to be valid in the three-level setup designed for nonadiabatic holonomic quantum computation proposed in Ref. [3] over a wide range system parameters. Only at small transition frequencies and very fast pulses does the RWA have an impact on the quantum systems evolution. The order of magnitude of state energy separation in atomic or molecular systems lies typically above this problematic region, already a separation of several meV is sufficient. Possible problems arising through the RWA can thus be avoided.

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