

Multi-Qubit Gates by Dynamical Decoupling Implemented with IBMQ and ^{15}NV Center in Diamond

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We demonstrate a general protocol for realizing fast high-fidelity multi-qubit gates, through dynamical decoupling (DD) pulse sequences applied to a central qubit coupled to target qubits. This way, we are able to control the states of the target qubits by leveraging their intrinsic interaction with the central qubit, eliminating the need for slow error-prone direct control. The DD-gate protocol is developed and experimentally implemented within two distinct frameworks: a hardware-agnostic model with minimal assumptions, benchmarked within a general-purpose digital quantum simulator given by the IBMQ; and an experimentally realistic case with nitrogen-15 vacancy center (^{15}NV) in diamond. Likewise, we are able to thoroughly characterize the quantum mechanical dynamics behind the multi-qubit gates within IBMQ, without many of the experimental constraints faced by other quantum systems. While at the same time, we establish the protocol for the ^{15}NV system, considering its specific properties. The DD-gates with ^{15}NV s can represent a significant reduction in gate times and improved technological scalability, compared to current methods of target qubit control using dynamical decoupling. In addition, we propose a simple application of the method for high-efficiency polarization generation of the ^{15}N nuclear spin. All experimental findings are supported by comprehensive open-source simulations in the two distinct frameworks. This work provides a robust hardware-agnostic strategy for quantum control, which can be implemented with arbitrary systems that fit the central-target qubits description. Thus, marking an essential step in technological scalability of future quantum devices.

I. INTRODUCTION

The generation of fast, reliable and technologically scalable multi-qubit gates is a fundamental challenge for quantum computing [1] and many other quantum technology applications [2–6]. A critical obstacle in this pursuit is the inherent trade-off between gate fidelity and operation time [7]. Here, we demonstrate a method that leverages dynamical decoupling (DD) [8] to mediate multi-qubit gates, simultaneously optimizing for speed and fidelity, while preserving technological scalability.

Our approach is designed but not restricted to a common architecture within quantum technology platforms: a central ‘control’ qubit that strongly interacts with external fields, coupled to one or more ‘target’ qubits with weak direct control. In such a way, coherent control of the central qubit is usually much faster and more precise than that of the coupled qubits. In contrast, the weakly interacting qubits generally have much longer coherence than the central qubit, placing them as ideal candidates for quantum memories [6, 9]. A primary example of such systems is color center defects in transparent solids [10, 11], which commonly have an electronic spin ($\hat{S}$) coupled to one or more nuclear spins ($\hat{I}$), where gate durations with the first are several orders of magnitude shorter than with the second [12]. Although direct excitation of the weakly interacting qubits by resonant pulses is possible [12], an

alternative that makes use of the fast high fidelity gates to the central qubit instead is highly desirable. Within this context, DD techniques can be a critical mean for exploiting the intrinsic interaction between the control and target qubits for realizing multi-qubit gates.

Pulsed DD sequences consist of periodic reversals of the quantum evolution of a qubit, such that environmental noises are canceled out from the total time evolution. In particular, the CPMG- N sequence [13] is composed of N repeated π_x pulses spaced with a free evolution of duration τ . $\pi_y/2$ pulses are also included before and after the sequence to drive the qubit from and to the quantization axis z . As the number of pulses N increases, the sequence acts as a narrow filter for frequencies corresponding to twice the inverse pulse separation $\omega = 1/(2\tau)$ and odd multiples of it [14, 15]. This resonance condition is schematically depicted in Fig. 1 (b). In the static laboratory frame, the target qubits perform Larmor precessions characterized by periodic oscillations of their expectation values $^{Lab}\langle\hat{I}\rangle(t)$, which average out to zero. But in the referential of the control qubit, the expectation value $^S\langle\hat{I}\rangle(t)$ adds up constructively if the pulse separation is in resonance with its Larmor frequency, while other signals with different frequencies cancel out destructively. In this way, by tuning the pulse separation with the resonant frequency of one of the target qubits, all other interactions in the system can be filtered from the control qubit, apart from the interaction with the target. Which in turn we utilize to perform gates to the target qubit, without the application of slow resonant pulses to them.

This application is notably well suited for color centers,

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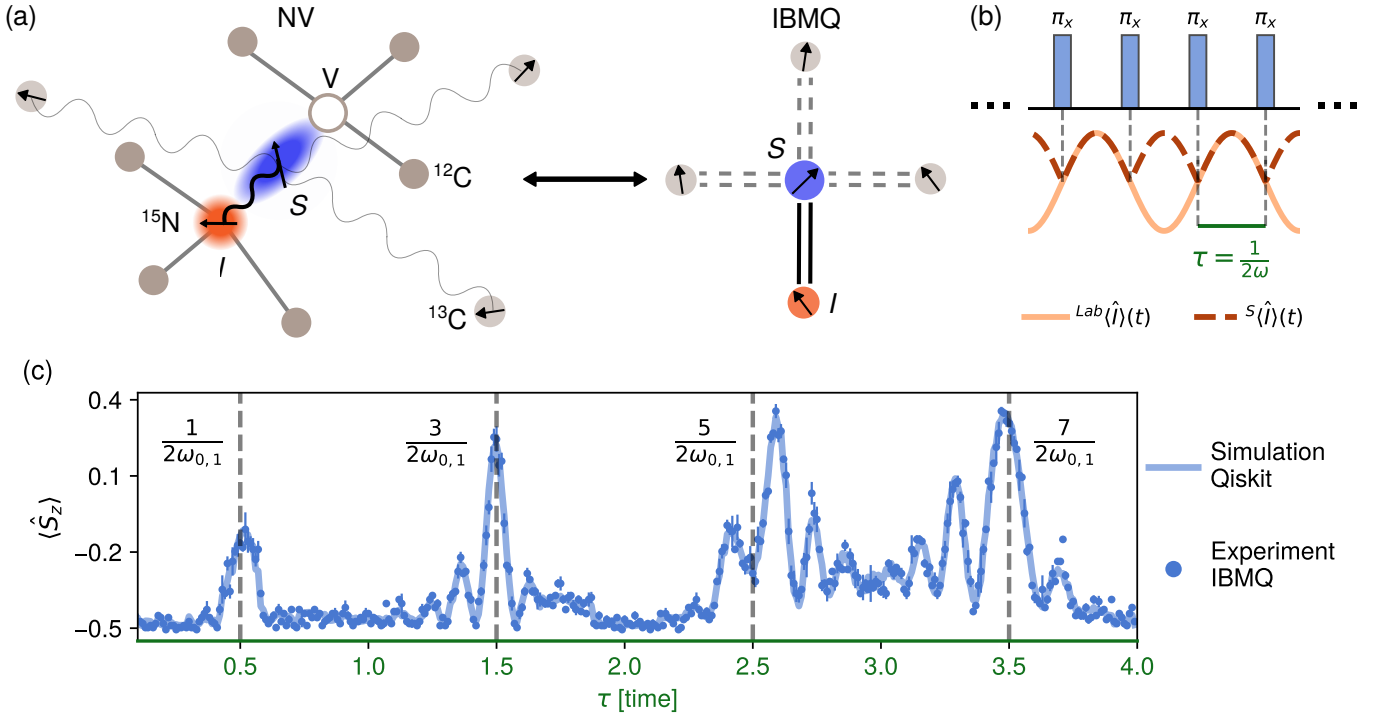


FIG. 1. **(a)** ^{15}NV center and IBMQ digital quantum simulator. ^{15}NV s defects in the diamond lattice are composed by an electronic spin S (control qubit), the ^{15}N nuclear spin I (target qubit) and a ^{13}C nuclear spin bath. The IBMQ is employed as a digital quantum simulator to emulate this dynamics, without the complex bath interaction and other experimental constraints. **(b)** CPMG dynamical decoupling sequence. By changing the separation τ between consecutive π_x -pulses to the control qubit, the sequence filters out signals which are not in resonance with the frequency $\omega = 1/(2\tau)$ and odd multiples of it. In this way, the target qubit expectation value $^{Lab}\langle\hat{I}\rangle(t)$ averages to 0 in the laboratory frame, but constructively adds up in the reference frame of the control qubit $^S\langle\hat{I}\rangle(t)$. **(c)** Experimental and simulated time-evolution of the target qubit under a CPMG-10 sequence in IBMQ. The $\langle\hat{S}_z\rangle$ observable shows resonances at the odd multiples of $1/(2\omega_{0,1})$, with pronounced sidebands at larger τ . An excellent agreement between the experimental and simulation data is observed.

due to the natural presence of both electronic and nuclear spins species. Specifically, we consider the nitrogen-vacancy (NV) center in diamonds [16, 17], composed of a substitutional nitrogen adjacent to a vacancy in the diamond lattice, as shown in Fig. 1 (a). NVs host an electronic spin $S = 1$ and a nitrogen nuclear spin $I = 1$ for the ^{14}N isotope (99.6% natural abundance) or $I = 1/2$ for ^{15}N (0.4%). In this study, we only consider the ^{15}NV center due to the absence of a quadrupole interaction, which suppresses the Larmor precession of the nuclear spin [18] (see Sec. III A). From now on, the ^{15}NV center is simply referred as NV. Apart from the nitrogen, the electron spin of the NV can also couple with spin-1/2 nuclei from ^{13}C atoms in the diamond lattice [19]. Where in this case, the DD sequences are used to decouple the ^{13}C spin bath and other paramagnetic noises from the NV electronic spin [20], such that the ^{15}N spin can be controlled.

Similar applications where ^{13}C nuclear spins are addressed with DD sequences applied to the NV electronic spin were already extensively studied [21–26], but in most cases relying on combined resonant radio-frequency (RF) pulses to the ^{13}C spins. In this work, we demonstrate

an unprecedented realization with the ^{15}N nuclear spin, without adoption of rotating frames and solely through microwave (MW) pulses to the electron spin. Using ^{15}N instead of ^{13}C has a critical technological advantage with regards to scalability, as the interaction Hamiltonian for a coupled ^{15}N is the same, independent of the NV. While ^{13}C nuclei are stochastically distributed in the diamond lattice around the NV (at current technological levels of material fabrication), which results in a varied number of possible Hamiltonians [27]. The technological scalability of such a method is particularly useful for diamond-based quantum token proposals [9, 28], where the nuclear spins are envisioned to store quantum states prepared using the electronic spin as an auxiliary qubit. In addition, our theoretical model goes beyond previous implementations, by allowing generalized coupling strengths that would not be suitable in perturbative approaches with adoptions of rotating frames, such as the rotating wave approximation.

Although particularly interesting for color centers, the use of DD of a control qubit for performing multi-qubit gates to target qubits can also be relevant to other qubit architectures, as superconducting qubits or quantum dots. It is thus indispensable to develop such a general non-

perturbative model for verifying the fundamental principles of the technique, while experimentally benchmarking it in a general-purpose quantum processor. With this goal, we employ IBM Quantum Platforms (IBMQ) as digital quantum simulators, composed of superconducting qubits [29–31]. Arguably, the most advanced cloud-based quantum processors available for public use. The IBMQ can thus emulate the behavior of an NV center [Fig. 1 (a)], or other general quantum systems, free from complex spin bath dynamics and other experimental constraints.

We begin this work in Sec. II introducing the minimal Hamiltonian model for multi-qubit DD mediated gates with generalized quantum systems, numerically simulated and experimentally realized in IBMQ through Qiskit software [32]. Built upon this general model, we then discuss its application with NV centers in Sec. III. Experimental measurements of the NV’s electron spin are shown and compared with simulations performed with QuacCAtoo software [33, 34]. An application of this technique for ^{15}N nuclear spin polarization is theoretically proposed, which could represent a significant simplification in experimental complexity, as compared to existing methods [7, 35]. Finally, we conclude in Sec. IV discussing the limitations and outlook of the model. The simulations and experimental implementations with IBMQ are open source, provided through a Python package available at [36]. In addition, the simulations of the NV center are provided at the QuacCAtoo repository [34].

II. UNIVERSAL MODEL BENCHMARKED ON IBMQ

To fully realize the multi-qubit gates by DD of the central qubit, we make use of the IBMQ Torino processor from the Heron family. Further experimental details are given in Appendix A 1, while Appendix B discusses the effect of the coupling factor A_{zx} . In Sec. II A, we introduce the theoretical framework for performing the time-evolution of the IBMQ system under the DD sequences. Following on that, in Sec. II B, we demonstrate the two-qubit gate of the central qubit coupled to one target qubit. In Sec. II C, we analyze the effects of pulse errors in the DD sequences. Finally, in Sec. II D, we realize a three-qubit gate with two target qubits, demonstrating the robustness of the DD method.

A. Theoretical Framework

A general system for multi-qubit gates by DD comprises the central qubit, represented by the quantum mechanical operators $\hat{\mathbf{S}} = (\hat{S}_x, \hat{S}_y, \hat{S}_z)$, and M target qubits, given by the operators $\hat{\mathbf{I}}_j = (\hat{I}_{x,j}, \hat{I}_{y,j}, \hat{I}_{z,j})$ with indices $j = 1, 2, \dots, M$. We adopt the suggestive notation of $\hat{S}_i$ and $\hat{I}_{i,j}$, given that the central qubit can be an electronic spin and the target a nuclear one. These quantum mechanical operators are taken as the spins operators

corresponding to Pauli matrices $(\hat{\sigma}_x, \hat{\sigma}_y, \hat{\sigma}_z)$ divided by the qubit dimension, which is 2 for a qubit. When considering the NV systems on the other hand, we analyze the dynamics with a spin-1 system (Sec. III). We take all qubits initialized in their state $|0\rangle$ and as having their quantization axis along z , with the central qubit having a Larmor frequency of $\omega_{0,0}$ determined by the energy difference between its states. While the target qubits have $\omega_{0,j}$ as their Larmor frequencies, being much smaller than the central qubit’s Larmor frequency $\omega_{0,j} \ll \omega_{0,0}$. We further consider that each target qubit has an coupling with the central qubit described by a 3×3 tensor $\mathbf{A}^j$ as $\hat{\mathbf{S}} \cdot \mathbf{A}^j \cdot \hat{\mathbf{I}}_j$, where the interaction between the target qubits is neglected.

Within these considerations, the system’s Hamiltonian can be written as

$$\hat{H}_0 = \omega_{0,0} \hat{S}_z + \sum_{j=1}^M \left(\omega_{0,j} \hat{I}_{z,j} + \hat{\mathbf{S}} \cdot \mathbf{A}^j \cdot \hat{\mathbf{I}}_j \right), \quad (1)$$

where we assume $\hbar = 1$ throughout this work, thus taking the Hamiltonians, coupling terms and frequencies in units of inverse time. For the generation of the multi-qubit gates, we are only interested in the coupling terms that involve the $\hat{S}_z$ and $\hat{I}_{x,j}$ components in the form of $A_{zx}^j \hat{S}_z \hat{I}_{x,j}$. This is because the central qubit can sense interactions along its quantization axis z [37], while the perpendicular components x and y cause qubit flips. Contrarily, in the target qubits, we are interested in these perpendicular components that will cause transitions between the states, where we only take the x component due to the freedom of choice of the coordinate system. Therefore, we have the minimal Hamiltonian model of

$$\hat{H}_0 = \omega_{0,0} \hat{S}_z + \sum_{j=1}^M \left(\omega_{0,j} \hat{I}_{z,j} + A_{zx}^j \hat{S}_z \hat{I}_{x,j} \right). \quad (2)$$

Strictly speaking, the interaction tensor $\mathbf{A}^j$ should be symmetrical and we would need to have terms with $A_{zx}^j \hat{S}_x \hat{I}_{z,j}$. However, these terms do not affect considerably the dynamics of the system under the DD sequences [38] and increase the computational costs with IBMQ, thus being neglected. NV centers exhibit a Hamiltonian model more complex than this one, but which still presents these same features, as discussed in detail in Sec. III A.

Having introduced the time-independent component of the Hamiltonian, we now need to model the interaction of the central qubit with the control field. Considering harmonic square pulses along the x direction [33], the time-dependent Hamiltonian in the laboratory frame during a pulse is given by

$$\hat{H}_1(t) = \omega_1 \cos(2\pi\omega_p t + \phi) \hat{S}_x, \quad (3)$$

where ω_1 is the Rabi frequency of the transition [39], ω_p is the frequency of the pulse and ϕ its phase. Taking the pulse in resonance with the central qubit $\omega_p = \omega_{0,0}$ will cause transitions between its two-levels, with ϕ controlling the rotation axis in the rotating frame. In addition,

assuming $\omega_{0,0} \gg \omega_1$, the expectation value of the central qubit $\langle \hat{S}_z \rangle$ will perform harmonic oscillations as a function of the pulse duration t_p , known as Rabi oscillations [40]. Taking a pulse length as $t_\pi = 1/(2\omega_1)$ will result in a complete inversion of the energy level populations, i.e. a π -pulse. In case $\omega_{0,0} \gg \omega_1$ is not valid, the qubit can also oscillate between its states, but not harmonically [41].

When considering single qubit dynamics, a rotating frame is typically adopted [42], such that the $\hat{H}_1(t)$ Hamiltonian becomes time-independent. However, the unitary transformation operator of the rotating frame does not necessarily commute with the Hamiltonian $\hat{H}_0$ from Eq. 1 depending on $\mathbf{A}^j$, which would then lead to time-dependencies in $\hat{H}_0$ in the rotating frame (as is the case with the NV Hamiltonian). Furthermore, the use of the rotating frame imposes that $\omega_{0,0} \gg A_{zx}^j$ and $\omega_{0,0} \gg \omega_1$, which are not always valid, or in the second case advantageous due to a slow driving of the central qubit. Altogether then, the most general approach for this problem is to realize the system dynamics within the quantum simulator in the static laboratory frame, differently from most quantum computing applications. This time-dependent description of the control Hamiltonian $\hat{H}_1(t)$ also allows us to directly account for pulse errors, as performed in Sec. II C.

Experimentally performing a free-evolution under $\hat{H}_0$ in the IBMQ processor at the laboratory frame is a straightforward operation. For that, the state of the system can be evolved with the time-evolution operator

$$\hat{U}_\tau = \exp \left[-i2\pi(\tau - t_\pi)\hat{H}_0 \right], \quad (4)$$

where $\tau - t_\pi$ is the actual pulse separation when considering realistic pulses with finite length [33]. The exponential operators are applied to the qubits through Pauli evolution gates [43], transpiled to the native gates of the hardware. More experimental details on the transpilation and execution of the circuits are given in Appendix A 1, while the exact implementation of the time-evolution gates are provided at [36].

If we wanted to theoretically solve the system dynamics during the pulse applications under the time-dependent Hamiltonian $\hat{H}_0 + \hat{H}_1(t)$, a Dyson series [44] could be used, involving an infinite sum of time integrals. But clearly, when considering this operation with a digital gate-based quantum simulator, the time variable cannot be continuously divided into infinitesimal components dt , infinitely integrated and summed. Instead, to achieve the pulse dynamics with IBMQ, we need to decompose the continuous time-evolution into a finite number of quantum gates. For that, we discretize the time-variable into small Δt steps and perform a product series of exponential operators in the form of

$$\hat{U}_p(t_p) \approx \prod_{k=1}^{t_p/\Delta t} \exp \left\{ -i2\pi\Delta t \left[\hat{H}_0 + \hat{H}_1(t_k) \right] \right\}, \quad (5)$$

ordered from right to left. This way, the operator ordering is explicitly handled in the IBMQ execution, with-

out requiring the time-ordering operator. For this approximation to be valid, Δt needs to be small compared to $1/\omega_{0,0}$, such that the Hamiltonian is nearly constant at the time t_k and it can be applied as if it was time-independent. However, even in the continuous case of the Dyson series, the perpendicular coupling terms and the time-dependent drive make a general analytical solution to the time-evolution operator unreachable.

By the end of the sequence, we assume that the central and target qubits can be measured through the quantum mechanical observables of their quantization axes $\hat{S}_z$ and $\hat{I}_{z,j}$. In this theoretical model, non-unitary processes such as decoherence and relaxation are not explicitly accounted for, which could be numerically incorporated through collapse operators in the Lindblad equation [33, 45]. But instead, they are included within the noise model of the IBMQ processors inside the Qiskit simulations framework (Appendix A 1). As will be seen in the following section, decoherence does not affect considerably the DD-gates with IBMQ at these time-scales, but does play an important role for NVs.

B. Two-Qubit Gate

We begin studying a simple case for the generation of the DD-gates with one single coupled spin. In this case, Eq. 2 becomes

$$\hat{H}_0 = \omega_{0,0}\hat{S}_z + \omega_{0,1}\hat{I}_z + A_{zx}\hat{S}_z\hat{I}_x, \quad (6)$$

where we simplify the notation by dropping the j index. We numerically take $\omega_{0,0} = 50$, and $\omega_{0,1} = 1$ in units of [time⁻¹]. The coupling factor A_{zx} is taken in the range from 0.05 to 1 depending on the measurements, ensuring that the Zeeman interaction of the target qubits is dominant over the coupling term $A_{zx} \leq \omega_{0,1}$. A complete analysis on the influence of the coupling factor on the DD gates is given in Appendix B. In the $\hat{H}_1(t)$ Hamiltonian (Eq. 3) we take $\omega_1 = 5$ [time⁻¹], such that $\omega_{0,0} \gg \omega_1$ is valid and the driving of the central qubit is harmonic [41]. Last, in Eq. 5, we adopt a time-step of $\Delta t = 0.001$ [time]. If we assume that the central qubit is an electronic spin and the target is a nuclear spin, the Larmor frequency of the central qubit is typically 10^3 to 10^4 times larger than the target qubits. But a large $\omega_{0,0}$ would require a small time step Δt , so that the $\hat{H}_1(t)$ Hamiltonian is nearly constant in each discretized time t_k in Eq. 5. Thus, to avoid increased computational costs in the IBMQ, we take this value of $\omega_{0,0}/\omega_{0,1} = 50$.

A CPMG sequence with $N = 10$ pulses was experimentally realized in IBMQ and simulated in Qiskit within these conditions and taking $A_{zx} = 0.1$ [time⁻¹], as shown in Fig. 1 (c). By varying the pulse separation τ , we observe that the central qubit observable $\langle \hat{S}_z \rangle$ has multiple resonances centered at the odd multiples of the fundamental resonant frequency: $1/(2\omega_{0,1})$, $3/(2\omega_{0,1})$, $5/(2\omega_{0,1})$ and $7/(2\omega_{0,1})$. These resonances also display sidebands,

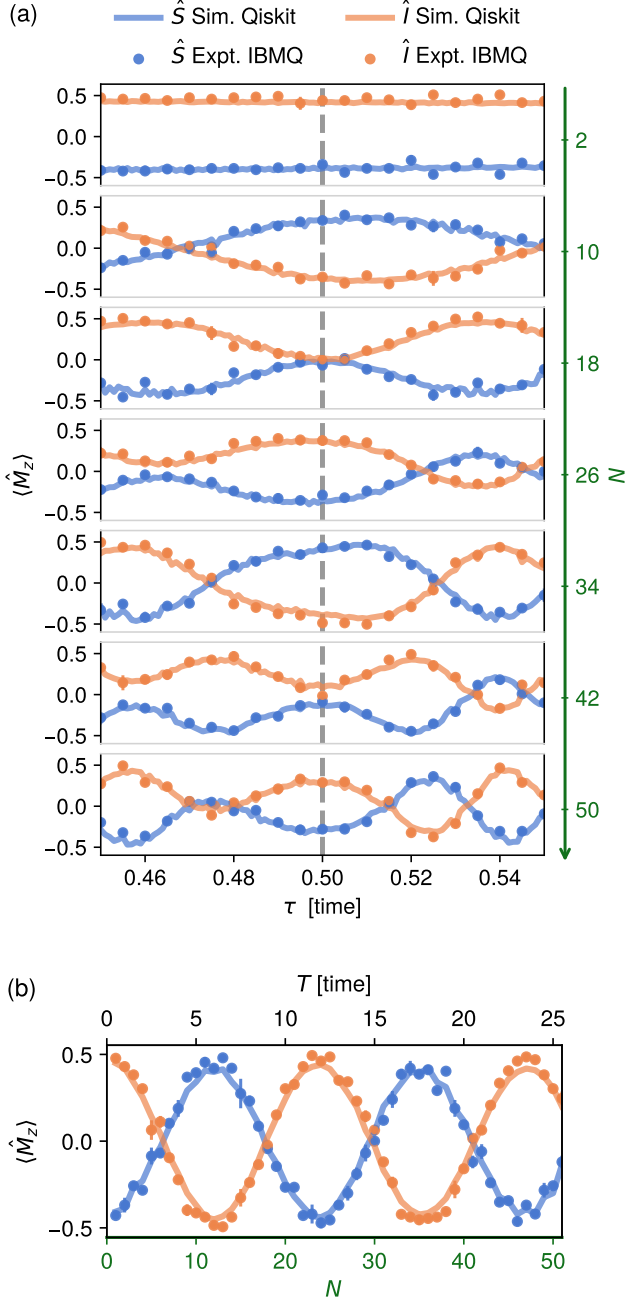


FIG. 2. (a) IBMQ experimental and simulated CPMG- N sequences applied to the control qubit. The target qubit observable $\langle \hat{I}_z \rangle$ has a time-evolution opposite to the control qubit $\langle \hat{S}_z \rangle$, with a resonance at $\tau = 1/(2\omega_{0,1}) = 0.5$ [time $^{-1}$]. As the number of pulses N increases, the amplitude of the resonance varies and sidebands become more pronounced. (b) Rabi-like oscillations of the two qubits. By taking $\tau = 0.5$ [time $^{-1}$] fixed and varying N , the two observables perform opposite harmonic oscillations, without observation of a signal decay from non-unitary process. This variation of the $\langle \hat{I}_z \rangle$ observable is the basis for the DD-gates.

more pronounced at the longer pulse separations. Notably, the simulation shows excellent agreement with the experimental data.

This method is broadly used for quantum sensing of coupled qubits [14, 15, 38], but in this case, our goal is to use the DD sequence resonances to control the time-evolution of the target qubit. To characterize the time-evolution dynamics of the target qubit, we take τ values around the first resonance at $\tau = 1/(2\omega_{0,1})$ and vary the number of pulses N , measuring both observables, as presented in Fig. 2 (a). Here, we take $A_{zx} = 0.2$ [time $^{-1}$] in order to achieve better resonance contrast (Appendix B). Again, we observe a strong agreement between the experimental data from IBMQ and the Qiskit simulation of the CPMG- N sequences. As the number of pulses increases, the filter function of the DD sequence changes [46], resulting in narrower resonance linewidths, with more pronounced sidebands and oscillations of the resonance amplitudes. Furthermore, the target qubit has a time-evolution under the DD sequence opposite to the central qubit, when considering this initial state $|0, 0\rangle$ (a case with a mixed initial state is discussed in Sec. III C). In this way, an increase in the resonance amplitude of the $\langle \hat{S}_z \rangle$ observable at some τ corresponds to a decrease by the same amount in the $\langle \hat{I}_z \rangle$ observable of the target qubit.

To further analyze this effect, we take $\tau = 0.5$ [time] fixed and measure the expectation value of the observables as a function of N in Fig. 2 (b). This shows that the central and target qubits observables $\langle \hat{S}_z \rangle$ and $\langle \hat{I}_z \rangle$ perform opposite harmonic oscillations with the same frequency and amplitude. The dependency of this oscillation frequency on the coupling factor is discussed in detail in Appendix B. Again, the experimental data shows strong agreement with the simulation, with no signal decay. Without the presence of non-unitary processes, these oscillations continue indefinitely without damping. Whereby taking $N = 12$ pulses, we have a complete inversion of both observables, totaling $T_\pi = N\tau = 6$ units of time, which can represent a considerable reduction in the gate duration as compared to direct excitation of the target qubit (see Sec. III B).

The oscillation of the observables suggests that the system is undergoing a Rabi oscillation [40] corresponding to rotations in the Bloch sphere for both qubits, but this is not case. By measuring the components $\langle \hat{I}_x \rangle$ and $\langle \hat{I}_y \rangle$ perpendicular to the quantization axis, we observe that in fact the qubits evolve from one pole of the Bloch sphere (state $|0\rangle$) to the other (state $|1\rangle$) through points inside the sphere, not on its surface as occurs with proper rotations. Fig. 3 (a) depicts this effect, by showing experimental data for N between 0 to 12 of the reduced density matrix corresponding to the subsystem of target qubit:

$$\hat{\rho}_I = \text{Tr}_S(\hat{\rho}) = \frac{\hat{1}}{2} + \sum_{a=x,y,z} \langle \hat{1} \otimes \hat{I}_a \rangle \hat{\sigma}_a, \quad (7)$$

where we explicitly write the tensor product of the target qubit observables.

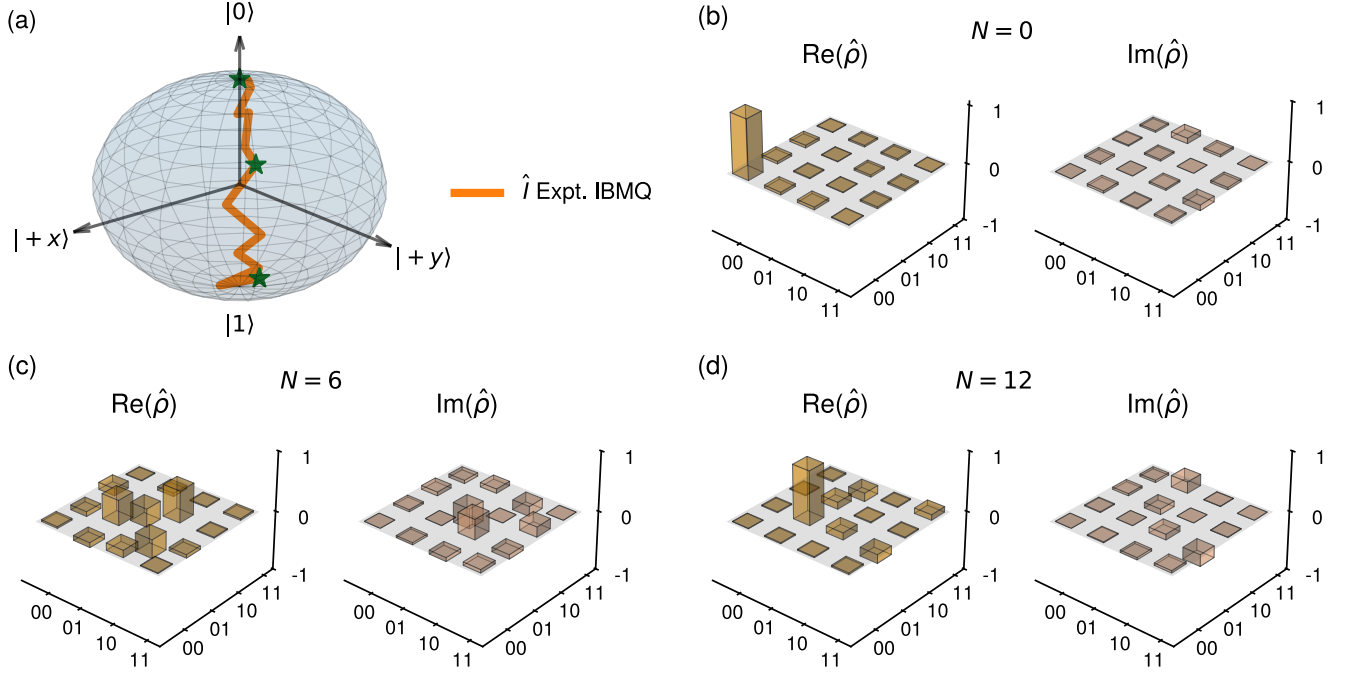


FIG. 3. (a) Bloch sphere representation of the target qubit under the experimental DD-gate with IBMQ. During the CPMG- N sequences, the subsystem state obtained from a partial trace of the two-qubits occupies points inside the sphere, which does not qualify the gate as proper rotation. Full density matrices $\hat{\rho}$ at (b) $N = 0$, (c) $N = 6$ and (d) $N = 12$ pulses, obtained from experimental quantum state tomography. These points are represented in (a) by the green stars. At $N = 0$ the system is well initialized in the $|00\rangle$ state, with small readout errors. In the middle of the gate at $N = 6$, the diagonal population term is distributed into off-diagonal terms representing entanglement, which results in mixed states for the single qubits when taking the partial traces of $\hat{\rho}$. At $N = 12$, the entanglement terms are reverted back into diagonal terms, resulting in a population inversion for the target qubit with fidelity 0.948, limited by the discretized nature of N .

When considering single qubits, the fact that the state is represented by a point inside the sphere would indicate a non-unitary dynamics, inducing state mixing. But with two qubits, this is not a valid interpretation, as the Bloch sphere is an incomplete description of the system. Specifically, the density matrix for a two-qubit system is

$$\hat{\rho} = \frac{\hat{\mathbb{1}}}{4} + \frac{1}{2} \sum_{a=x,y,z} \left(\langle \hat{S}_a \otimes \hat{\mathbb{1}} \rangle \hat{\sigma}_a \otimes \hat{\mathbb{1}} + \langle \hat{\mathbb{1}} \otimes \hat{I}_a \rangle \hat{\mathbb{1}} \otimes \hat{\sigma}_a \right) + \sum_{a,b=x,y,z} \langle \hat{S}_a \otimes \hat{I}_b \rangle \hat{\sigma}_a \otimes \hat{\sigma}_b.$$

Where only the first line is fully expressed in the Bloch spheres, thus averaging out the entanglement terms with $\langle \hat{S}_a \otimes \hat{I}_b \rangle$. It is not surprising then that by taking a partial trace of the whole system (Eq. 7), the qubit subsystems are in mixed states. More interestingly, this shows that the initial population of the $|0,0\rangle$ state is distributed into the off-diagonal terms of the density matrix representing entanglement, which are not represented by the Bloch sphere. And after a certain number of pulses, the off-diagonal terms evolve back into population terms, resulting in a population inversion to the $|0,1\rangle$ state. This behavior is evidenced by the experimental full quantum state tomography with the 15 observables [47] for $N = 0$

(initial state preparation) $N = 6$ (intermediate ‘ $\pi/2$ ’ state) and $N = 12$ (final ‘ π ’ state) in Figs. 3 (b), (c) and (d) respectively. At $N = 0$, the IBMQ shows a nearly perfect initialization of the qubits, with small deviations in some of the off-diagonal terms, likely due to readout errors related to the rotations necessary for the projection into the measurement axis. While at $N = 12$, we observe a complete population inversion of the target qubit. By taking an intermediate number of pulses as $N = 6$, we obtain a highly entangled state with concurrence 0.899 [48, 49], close to a maximally entangled state with concurrence 1. In this way, the DD-gates can potentially be employed as tool for entanglement generation, apart from population changes to the target qubits, which motivates further research into this time-evolution dynamics.

At the final state, small deviations from a perfect population inversion of the target qubit are also observed. This can be attributed to the readout errors as seen at $N = 0$ and the time discretization Δt , which can further introduce errors. But mainly, this discrepancy is related to the discrete nature of the N variable, which does not allow us to take the exact moment during the time evolution where the state is completely inverted. The experimental final state fidelity with the ideal $|0,1\rangle$ state is 0.945. But if we disregard the control qubit (which serves more

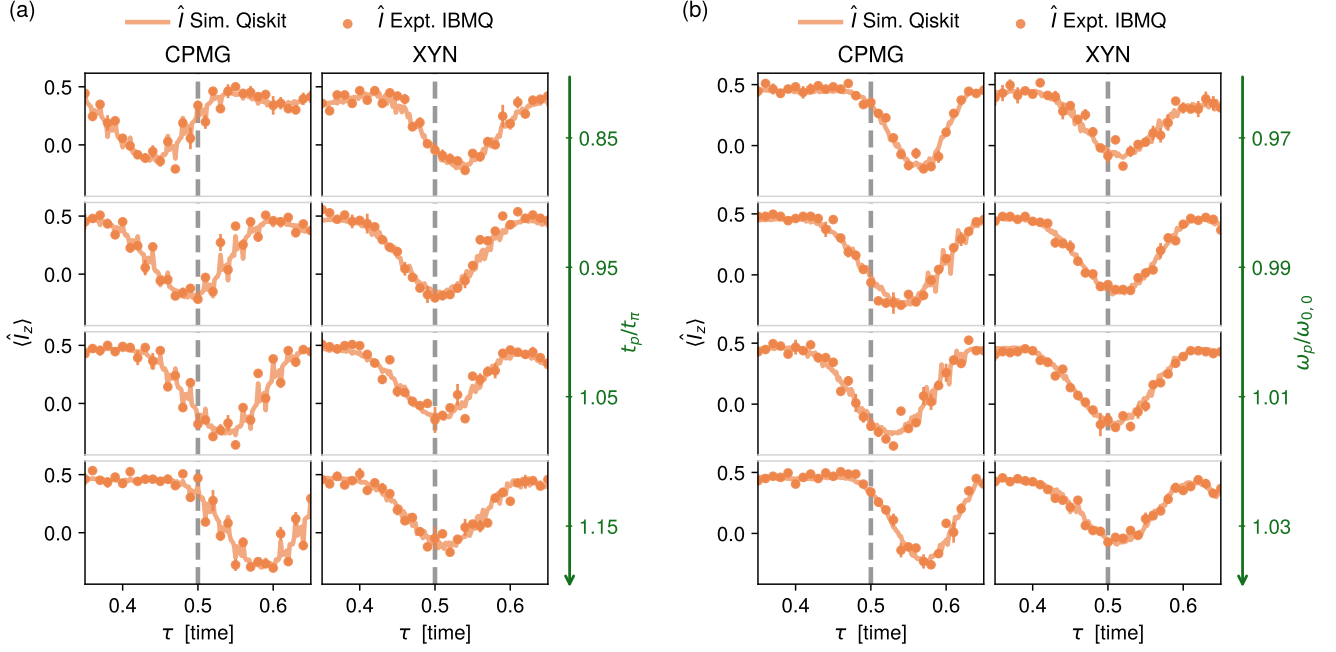


FIG. 4. IBMQ simulated and experimental CPMG-8 and XY8 sequences under (a) pulse length error t_p/t_π and (b) pulse frequency error $\omega_p/\omega_{0,0}$. Both frequencies present the same resonance feature, but as the pulse errors become larger, the CPMG resonances shift in τ . An effect which is not so prominent in the XYN sequence, evidencing a more robust pulse error resilience. Small periodical spikes are also observed in the CPMG [37, 41], demonstrating the robustness of the laboratory frame model, beyond the adoptions of rotating frames via perturbative approximations [37, 41].

as an auxiliary qubit) and take the partial trace of the system (Eq. 7), the fidelity for a population inversion of the target qubit is 0.995. Another metric which is related to this fidelity is the amplitude of the Rabi-like oscillation, denoted as the pseudo-fidelity $\tilde{F}$. Which for the experimental data in Fig. 2 (b), we have $\tilde{F} = 0.963$. This pseudo-fidelity has the advantage of not requiring a full quantum state tomography as performed here, thus being less computationally costly for IBMQ and utilized from now on.

C. Pulse Errors Resilience

An important factor which appears when dealing with multipulse DD sequences are errors in the control field, as they accumulate with each pulse until impairing the application of the sequence. Here, we consider two types of pulse errors in the control field (Eq. 3): duration of the pulse in regards to a perfect π -pulse duration t_p/t_π , and the frequency of the pulse as compared to the resonance of the central qubit $\omega_p/\omega_{0,0}$.

Although the CPMG sequence is one of the most widely used DD sequences, it is particularly prone to such errors [46]. This happens because the π -pulse is repeatedly applied over the same x axis, causing errors to accumulate fast. A natural improvement then to the CPMG sequence is to intercalate the N π -pulses between the

x and y axis [8, 50], which we denominate as XYN sequence. Notably, the XY8 sequence is widely used in quantum sensing applications [15, 37], being composed of eight intercalated pulses anti-symmetrized: $[\pi_x, \pi_y, \pi_x, \pi_y, \pi_y, \pi_x, \pi_x, \pi_y, \pi_x]$. In this application however, we do not anti-symmetrize the pulses to simplify the experimental realization of the DD-gate. Thus an XY8 sequence in this work is composed of $[\pi_x, \pi_y, \pi_x, \pi_y, \pi_x, \pi_y, \pi_x, \pi_y]$.

To compare the CPMG and XYN sequences under different pulse errors, we experimentally measured and simulated the target qubit observable $\langle \hat{I}_z \rangle$ in both sequences with $N = 8$ pulses. The same Hamiltonian as in Eq. 6 was used with coupling term of $A_{zx} = 0.2$ [time]. The effect in the sequences of pulse length errors from $0.85 t_p/t_\pi$ to $1.15 t_p/t_\pi$ while keeping the correct frequency $\omega_p/\omega_{0,0}$ are shown in Fig. 4 (a). While Fig. 4 (b) shows the sequences under pulse frequency errors from $0.97 \omega_p/\omega_{0,0}$ to $1.03 \omega_p/\omega_{0,0}$, while keeping the correct pulse duration $t_p = t_\pi$. Primarily, at small values of errors, both sequences have the same resonance feature at $\tau = 0.5$ [time], as expected [50]. However, as either errors increase, the position of the resonance shifts and the amplitude decreases with the CPMG sequence. An effect which is not so pronounced in the XYN sequence, indicating a more robust pulse errors resilience.

Another interesting effect can be observed in the CPMG sequence with pulse length errors. The experimental data and the simulations show small periodical spikes in the

resonance peak, similar to as observed in Ref. [37] and when the rotating wave frame approximation and adoption of the rotating frame are no longer valid [41]. Overall, this attests the robustness of this simple model in the laboratory frame, which can describe in excellent agreement with experiments the behavior of the DD sequences even in the presence of pulse errors. This incorporation of pulse errors could not be so straightforward or robust under the adoption of rotating frames and rotating wave approximations. It could be argued that a shift in the resonance could easily be corrected by adjusting the fixed τ value for the DD-mediated gate. However, pulse errors are not generally known prior to the application of the DD sequences. The assumption of previously knowing the shift to be applied in τ would thus be a design flaw in the pulse sequence of the DD-gate.

To further characterize the pulse error resilience of

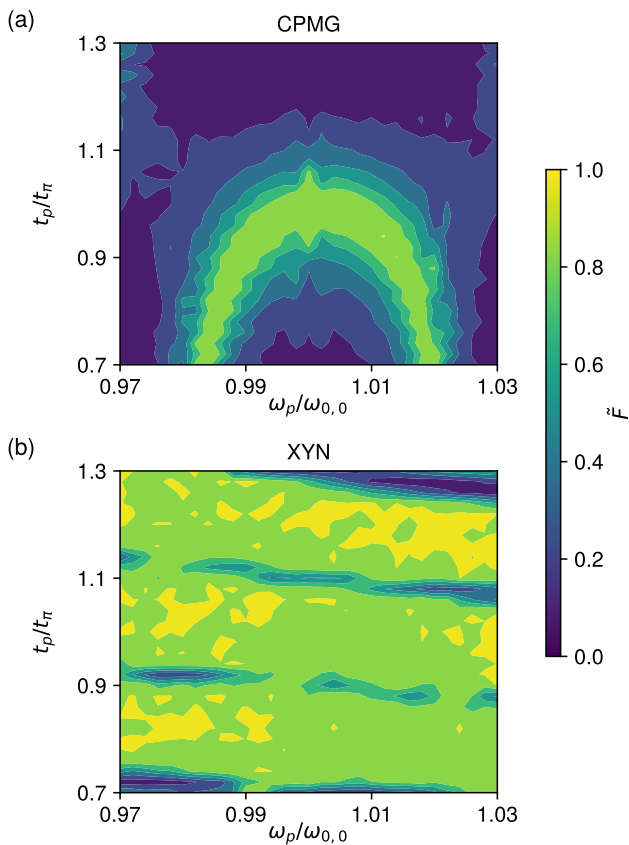


FIG. 5. Simulated pseudo-fidelity $\tilde{F}$ of the DD-gate as a function of pulse errors in IBMQ with (a) CPMG and (b) XYN sequences. The CPMG sequences shows a pronounced susceptibility to pulse errors, where small deviations in the control field lead to a substantial decrease of $\tilde{F}$, with a characteristic upside down ‘U’ shape [55]. The XYN sequence on the other hand represents a much more robust pulse error resilience, simply by intercalating the π -pulses in the x and y axes. This error resilience could be further improved with anti-symmetrization of the axis [50], addition of random phases [51–53], uneven pulse separation [54] or composite pulses [55].

the two sequences, we simulate them for several combinations of t_p/t_π and $\omega_p/\omega_{0,0}$, varying N and keeping $\tau = 0.5$ [time] fixed. This results in a series of Rabi-like oscillations as in Fig. 2 (b), from which we calculate the pseudo-fidelity $\tilde{F}$ of the DD-mediated gate, given by the amplitude of the oscillation (Sec. II B). The results as shown in Fig. 5 evidence a massive improvement in pulse error resilience in the XYN as compared to the CPMG. Whereby simply intercalating the excitation axis in the XYN sequence, pseudo-fidelities above 0.7 can be achieved throughout the considered error values of $0.7 t_p/t_\pi$ to $1.3 t_p/t_\pi$ and $0.97 \omega_p/\omega_{0,0}$ to $1.03 \omega_p/\omega_{0,0}$. Contrastingly, the CPMG sequence suffers from a great reduction in pseudo-fidelity, even with small deviations from the resonant conditions, with a characteristic upside down ‘U’ shape, as observed in other pulse errors resilience studies with IBMQ [55].

Given this more robust pulse errors resilience, the XYN is utilized for the realization of the DD-gate with the NV (Sec. III B), where the experimental design is much more susceptible to pulse errors than with IBMQ. But apart from being more robust, the XYN sequence produces a distinct filtering function as compared to the CPMG. This difference is further characterized in Sec. III C, where the CPMG and XYN sequences evidence contrasting dynamics with initially mixed states. Apart from the anti-symmetrization of the pulses, the pulse errors resilience of the XYN sequence for the DD-gate could be further improved with the addition of random phases in each $[\pi_x, \pi_y, \pi_x, \pi_y]$ block [51, 52], where the random phases can be correlated for even better error suppression [37, 53]. Beyond that, asymmetrical pulse separation can be introduced as in Uhrig DD [54], or composite pulses can be considered [55].

D. Three-Qubit Gate

To ascertain the robustness of the decoupling and benchmark the model to multiple target qubits, we perform the DD-gate in a three qubits system, composed by the central qubit coupled with two target qubits, as schematically represented in Fig. 6 (a). We consider a Hamiltonian as in Eq. 1, with the same parameters for the control qubit as in Sec. III B and target qubits parameters of $A_{zx,1} = 0.15$, $A_{zx,2} = 0.10$, $\omega_{0,1} = 1$ and $\omega_{0,2} = 0.5$, all in units of $[\text{time}^{-1}]$. In addition, we take a smaller time-step of $\Delta t = 0.0001$, in order to achieve a better approximation with the time discretization of the Pauli operators (Eq. 5).

First, we experimentally measured and simulated the expectation values of the three qubits $\langle \hat{S}_z \rangle$, $\langle \hat{I}_{z,1} \rangle$ and $\langle \hat{I}_{z,2} \rangle$ under a CPMG-10 sequence, as shown in Fig. 6 (b). Each of the two target qubits show a resonance at their Larmor frequencies $\tau = 1/(2\omega_{0,j})$, without having any response at the other target qubit’s resonant pulse separation. The central qubit displays the resonances at both of the frequencies, which can make it difficult for spectral

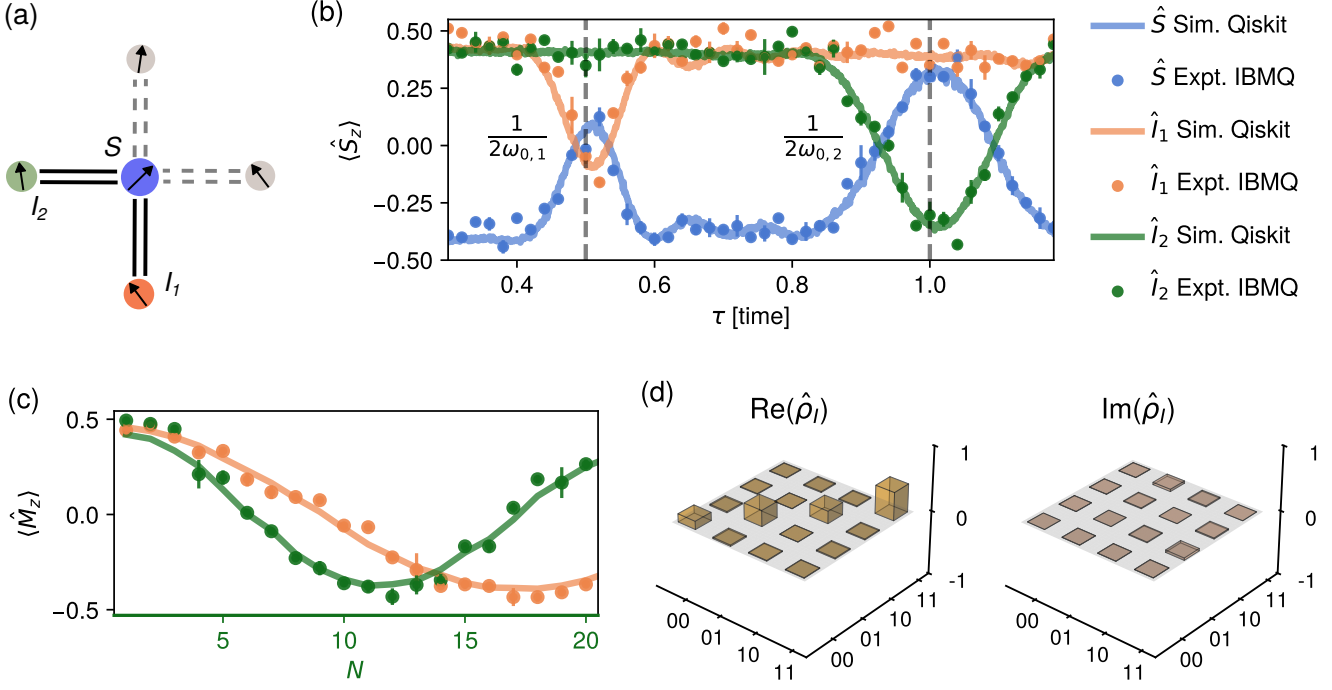


FIG. 6. (a) Three-qubit representation scheme with IBMQ. The central control qubit is coupled to two target ones, with Larmor frequencies $\omega_{0,1} = 1$ and $\omega_{0,2} = 0.5$ [time⁻¹]. (b) Experimental and simulated CPMG-10 sequence applied to the central qubit in the three-qubits system. The central qubit observable $\langle \hat{S}_z \rangle$ shows resonances at both of the target qubits resonant τ values, while each of the target qubits has its own resonance determined by $\tau = 1/(2\omega_{0,j})$. (c) Experimental and simulated DD-mediated gates obtained with τ fixed to each qubit's resonance. The expectation values show an expressive signal decay, evidencing a limitation of the IBMQ digital quantum simulator to represent the central-targets qubits system under time-dependent pulses. (d) Experimental tomography of the reduced density matrix of the target qubits, with a partial trace over the control qubit. By applying a CPMG-16($\tau = 0.5$) sequence followed by a CPMG-11($\tau = 1.0$), both target qubits populations are inverted with a low fidelity of 0.659 as compared to the ideal state $|11\rangle$, while taking a partial trace of the control qubit. The poor performance of the DD-gate protocol with three qubits evidence a fundamental limitation for a digital gate-based quantum simulator to emulate a time-dependent Hamiltonian.

disambiguation in quantum sensing applications with DD sequences [37, 38].

To realize the DD-gate with the target qubits, the resonant pulse separation of each one is separately addressed with the CPMG sequence varying N , as previously done in Fig. 2 (b). The experimental and simulation results for the target qubits DD-gates are shown in Fig. 6 (c), demonstrating full population inversions at $N = 16$ in the target qubit 1 and $N = 11$ in qubit 2. An expressive signal decay is also observed in both of the observables, evidencing a limitation of the IBMQ digital quantum simulator to reproduce the model for three qubits. These signal decays are also present in the Qiskit simulations, in good agreement with the experiment, which validates the noise model employed in the simulations of the superconducting hardware.

The fidelities of each target qubit DD-gate is obtained by an experimental quantum state tomography, as done in Fig. 3. For the target qubit 1, the resulting fidelity in relation to the ideal state $|10\rangle$ is 0.702, where we take the partial trace of the control qubit. Whereas in target

qubit 2, we obtain 0.695 compared to the state $|01\rangle$. Both of these small values of fidelity are severely limited by the signal decay of the DD time-evolution. Finally, the two DD-gates can be composed together in the form of CPMG-16($\tau = 0.5$) + CPMG-11($\tau = 1.0$) to have a double population inversion of the two states yielding $|11\rangle$. In this case, we obtain a fidelity of 0.659, again taking the partial trace of the control qubit. The reconstructed density matrix for this final state is shown in Fig. 6 (d).

Such a poor performance of the the three-qubit gate is not necessarily an indicative of a limitation in the conceptualization of the theoretical model or some hardware imperfection. Instead, the low fidelities are fundamentally limited by the intrinsic time-dependent nature of the Hamiltonian. Which cannot be properly executed using a discrete set of quantum gates within the IBMQ quantum simulator, at current technological development levels of the hardware and the cloud-based execution services. This does not imply, however, that the DD mediated gate is not suitable for multi-qubit systems. As other architectures which are better suited with the central-

target qubits description than the IBMQ hardware can potentially present significantly improved performance.

III. EXPERIMENTALLY REALISTIC MODEL WITH ^{15}N

Among the various physical platforms utilized in quantum technologies, the NV center in diamond has been a focal point of research [16, 17], with applications ranging from quantum sensing [2–4], to networks [5] and memory-tokens [6, 9]. Apart from other qualities, the NV closely corresponds to the description of a central qubit coupled to a target one, as developed in Sec. II. In this section, we thus extend the minimal model developed and benchmarked with IBMQ for the NV system. In Sec. III A, we introduce the NV Hamiltonian and the simulation framework. Following that, in Sec. III B, we present experimental measurements of the electron spin and simulations of the nuclear spin for the DD-mediated gate. Finally, in Sec. III C, we discuss a possible application of the DD-gate for the polarization of the nuclear spins from an initial maximally mixed thermal state, supported by simulations. Further details on the experimental realization with NVs can be found at Appendix A 2, while the simulations of the DD-gates with NVs are provided in the QuaCCAToo tutorials section [34].

A. Theoretical Framework

In order to describe the time-evolution of the NV system under a DD sequence, we use a Hamiltonian model [56–58] for the electron spin operator $\hat{\mathbf{S}}$ and the ^{15}N nuclear spin $\hat{\mathbf{I}}$. Taking the z -axis aligned with the NV crystal axis, it can be written as

$$\hat{H}_0 = D\hat{S}_z^2 - \gamma^e \mathbf{B}_0 \cdot \hat{\mathbf{S}} - \gamma^n \mathbf{B}_0 \cdot \hat{\mathbf{I}} + A_{xx}\hat{S}_x\hat{I}_x + A_{yy}\hat{S}_y\hat{I}_y + A_{zz}\hat{S}_z\hat{I}_z. \quad (8)$$

The first term represents a zero-field splitting due to the dipolar coupling between the two electrons forming the electronic spin, with $D = 2.87$ GHz. The second and third terms are the Zeeman interactions with the external field $\mathbf{B}_0$, where the gyromagnetic ratios of the two spins are $\gamma^e = -28.025$ GHz/T and $\gamma^n = -4.316$ MHz/T. At magnetic fields below $|\mathbf{B}_0| < 102.4$ mT, the zero-field interaction is dominant over the electron Zeeman term and the lowest energy state corresponds to the $m_S = 0$ level. The last three terms correspond to the hyperfine interaction between the two spins, with $A_{xx} = A_{yy} = 3.65$ MHz and $A_{zz} = 3.03$ MHz [59], which in the principal axis system (PAS) aligned with the NV crystal axis corresponds to a diagonal coupling tensor $\mathbf{A}$.

In most applications, the external field is assumed to be parallel to the quantization axis $\mathbf{B}_0 \parallel z$, resulting in Zeeman interactions in the form of $-\gamma^e B_0 \hat{S}_z$ and $-\gamma^n B_0 \hat{I}_z$. However, as recently shown [37], a small misalignment

of $\mathbf{B}_0$ with the NV-axis can lead to a detection of the ^{15}N nuclear spin precession by the electronic spin in DD sequences. Assuming a small misalignment angle of θ_0 and adopting a reference frame in which $\phi_0 = 0$, the Zeeman terms become

$$\begin{aligned} -\gamma^e \mathbf{B}_0 \cdot \hat{\mathbf{S}} &= -\gamma^e B_0 (\cos \theta_0 \hat{S}_z + \sin \theta_0 \hat{S}_x) \\ -\gamma^n \mathbf{B}_0 \cdot \hat{\mathbf{I}} &= -\gamma^n B_0 (\cos \theta_0 \hat{I}_z + \sin \theta_0 \hat{I}_x) \end{aligned}$$

If θ_0 and $\mathbf{B}_0$ are too large, such that $|\gamma^e \mathbf{B}_0 \sin \theta_0| \sim D$, these relations are no longer valid, as the basis states for the electronic spin become hybridized [60]. In the context of quantum sensing, the presence of the perpendicular $\hat{S}_x$ term gives rise to ambiguous resonances in DD spectrum, which can be confused with the signal intended to be measured. But here, these resonances are the means for the DD-mediated nuclear gates. When considering the ^{14}N isotope on the other hand, a quadrupole interaction fixes the nuclear spin, suppressing its precession and making the application of such DD gates less practical.

The NV Hamiltonian under these considerations does not immediately resemble the minimal two qubits Hamiltonian, as in Eq. 6. But, by making the substitutions

$$\begin{aligned} D\hat{S}_z^2 - \gamma^e B_0 (\cos \theta_0 \hat{S}_z + \sin \theta_0 \hat{S}_x) &\longleftrightarrow \omega_{0,0} \hat{S}_z \\ -\gamma^n B_0 (\cos \theta_0 \hat{I}_z + \sin \theta_0 \hat{I}_x) &\longleftrightarrow \omega_{0,1} \hat{I}_z \\ A_{xx}\hat{S}_x\hat{I}_x + A_{yy}\hat{S}_y\hat{I}_y + A_{zz}\hat{S}_z\hat{I}_z &\longleftrightarrow A_{zx}\hat{S}_z\hat{I}_x, \end{aligned}$$

we result in a similar equation, with two important distinctions. First, the central spin is not a qubit, but rather a qudit of dimension 3, given that $S = 1$. This does not significantly affect the dynamics of the DD-gates as presented in Sec. II, provided that the energy splitting between $m_S = -1$ and $m_S = +1$ is much larger than the bandwidth of the central qudit pulses, in order to avoid double quantum excitations of the two electronic levels [61]. If this condition is met, the three-level system can effectively be treated as a qubit. The second and most important distinction is that the perpendicular term responsible for the central spin flips during the DD sequence is present in the Zeeman interaction and not the hyperfine coupling. To show that these terms are the physical manifestation of the same effect, we can assume a new reference frame along the $\mathbf{B}_0$ field, where now the NV axis is misaligned. In this new frame, the hyperfine coupling tensor is given by

$$\mathbf{A}' = \begin{pmatrix} A'_{xx} & 0 & A'_{xz} \\ 0 & A_{yy} & 0 \\ A'_{zx} & 0 & A'_{zz} \end{pmatrix}$$

with the new elements as

$$\begin{aligned} A'_{xx} &= A_{xx} \cos^2 \theta_0 + A_{zz} \sin^2 \theta_0 \\ A'_{zz} &= A_{xx} \sin^2 \theta_0 + A_{zz} \cos^2 \theta_0 \\ A'_{xz} &= A'_{zx} = (A_{xx} - A_{zz}) \sin \theta_0 \cos \theta_0, \end{aligned}$$

while A_{yy} remains the same. Clearly then, in this new referential, we have the presence of a A'_{zx} term responsible for DD resonances, as in the model developed for IBMQ. Although this referential is useful for qualitatively understanding the DD resonances with the ^{15}NV system, it can be computationally more expensive to simulate than in the PAS frame aligned with the NV axis. Therefore, we use the PAS frame for the simulations

Prior to the application of the DD sequences, the electronic spin of the NV is initialized into the state $|0\rangle \equiv |m_S = 0\rangle$ by an optical pumping mechanism [62] with the application of a green laser. In general, the ^{15}N nuclear state is in an initial mixed thermal state, with a density matrix practically equal to identity $\hat{1}/2$ [33], unlike the electronic spins and the IBMQ system. The nuclear spin can be polarized through projective measurements via the electron spin [35], yet this requires precise alignment of the $\mathbf{B}_0$ field with the NV axis, which we do not perform in this study. Overall then, the state of the NV system is described by mixed density matrices, rather than pure ket states. The control field interaction with the NV system, given by the time-dependent $\hat{H}_1(t)$ Hamiltonian, is analogous to Eq. 3. With the only difference being that due to the spin dimension $S = 1$, we select the $m_S = 0 \rightarrow -1$ transition frequency for the control pulse, with $|1\rangle \equiv |m_S = -1\rangle$ forming then the computational basis.

When considering the interaction of the NV's electron spin and surrounding ^{13}C nuclei, the hyperfine term is typically smaller or in the same order of the nuclear Zeeman interaction. This permits to calculate the DD resonance features in an analytical framework, based on the adoption of rotating frames and assumption of rotating wave approximations [23–26, 38]. For this case however, with the ^{15}N nuclear spin, the hyperfine term is dominant over the nuclear Zeeman interaction for moderate magnetic fields $\gamma_n|\mathbf{B}_0| > A_{xx}, A_{zz}$ and the break of symmetry of the misaligned $\mathbf{B}_0$ introduces non-commuting terms with the rotation operators of the rotating frame [63], making an analytical solution unfeasible. The dynamics of the system under the $\hat{H}_0 + \hat{H}_1(t)$ Hamiltonian then needs to be solved in the static laboratory frame with the Liouville-von Neumann equation [64], motivating the choice of this frame in Sec. II A. To numerically simulate this dynamics, we use the Quantum Color Centers Analysis Toolbox (QuaCCAToo) [33, 34] software, based on QuTip [65, 66], which is a more complete tool for simulating color centers systems than Qiskit.

At the end of the pulse sequence, we measure the fluorescence observable given by $\langle \hat{F} \rangle \equiv \text{Tr}(2\hat{\rho}_0\hat{\rho}_f)$ [33], where $\hat{\rho}_f$ is the final state of the system. With this definition, $\langle \hat{F} \rangle$ is related but not strictly the same as the expectation value of the $\hat{S}_z$ operator, as the $m_S = \pm 1$ states occupation cannot be distinguished by the emitted fluorescence. Since we are exciting just one of the electronic levels, both coincided and we refer to $\langle \hat{F} \rangle$ simply as the expectation value of the spin operator $\langle \hat{S}_z \rangle$. As for the ^{15}N nuclear spin observable, we assume the $\langle \hat{I}_z \rangle$ observable

as in Sec. II A. Noting, however, that $\hat{S}_z$ has expectation values from 0 to 1 in this definition, while $\hat{I}_z$ has from -0.5 to 0.5.

B. Realization of ^{15}NV DD-Gate

In order to characterize the DD resonance spectrum of a ^{15}NV in a misaligned magnetic field, a single center was measured under a magnetic field of $|\mathbf{B}_0| = 32$ mT and misalignment angle with the NV axis of $\theta_0 = 2.9^\circ$. The XYN sequence was chosen instead of the CPMG, given its more robust pulse errors resilience, as demonstrated in Sec. II C. Further experimental details are given in Appendix A 2. The experimentally measured and simulated expectation values of the electron spin observable $\langle \hat{S}_z \rangle$ for different values of pulses N are shown in Fig. 7 (a). The remaining values of N can be found at [34]. For comparison, we also show the simulated data for the nuclear spin observable $\langle \hat{I}_z \rangle$. While the direct experimental measurement of the nuclear spin polarization was not feasible in this work, the simulations provide valuable insight into the underlying system dynamics. We further assume an initially polarized state $|00\rangle = |m_S = 0\rangle \otimes |m_I = +1/2\rangle$, even though this does not strictly corresponds to the conditions of the experiment. Nonetheless, as observed in Sec. III C, the central spin observable is not affected by the initial state of the coupled spin under the XYN sequence.

A prominent resonance from the ^{15}N nuclear spin can be observed at around $\tau = 0.364$ μs , in accordance with Ref. [37]. Contrastingly to IBMQ, its position does not correspond to $\tau = 1/(2|\gamma_n\mathbf{B}_0|)$, given that the hyperfine coupling is dominant $|A_{zx}| > |\gamma_n\mathbf{B}_0|$ and the nuclear spin has a different Larmor frequency for each electronic level. As the number of pulses N increases, the filter function of the DD sequence is affected, making the linewidth of the resonances smaller due to an improved frequency filtering [46] and leading to the appearance of sidebands, as seen in Sec. II B. The intensity of the resonances also changes with N , where the DD mediated gate can be obtained by taking $\tau = 0.364$ μs fixed and varying N . The expectation values of $\langle \hat{S}_z \rangle$ perform the Rabi-like oscillations, analogous to Fig. 2 (b), where a complete inversion of the population can be obtained with 24 pulses, totaling $T_\pi = 9.04$ μs . This value is close to 100 times faster than the value reported in Ref. [38] for a ^{13}C nuclear spin, given the much stronger hyperfine interaction.

The QuaCCAToo simulations of the electronic spin observable show a good agreement with the experimental data for small values of N . However, as the sequence becomes longer, decoherence and pulse errors start to affect the experimental data, leading to a deviation from the simulation, as similarly observed in other DD sequences under pulse errors [37]. In this way, the NV cannot complete a whole 2π cycle of the DD-gate before the signal decays, a much worse scenario than observed with IBMQ. The pulse error resilience of the DD-gate can still be significantly improved in multiple ways, as

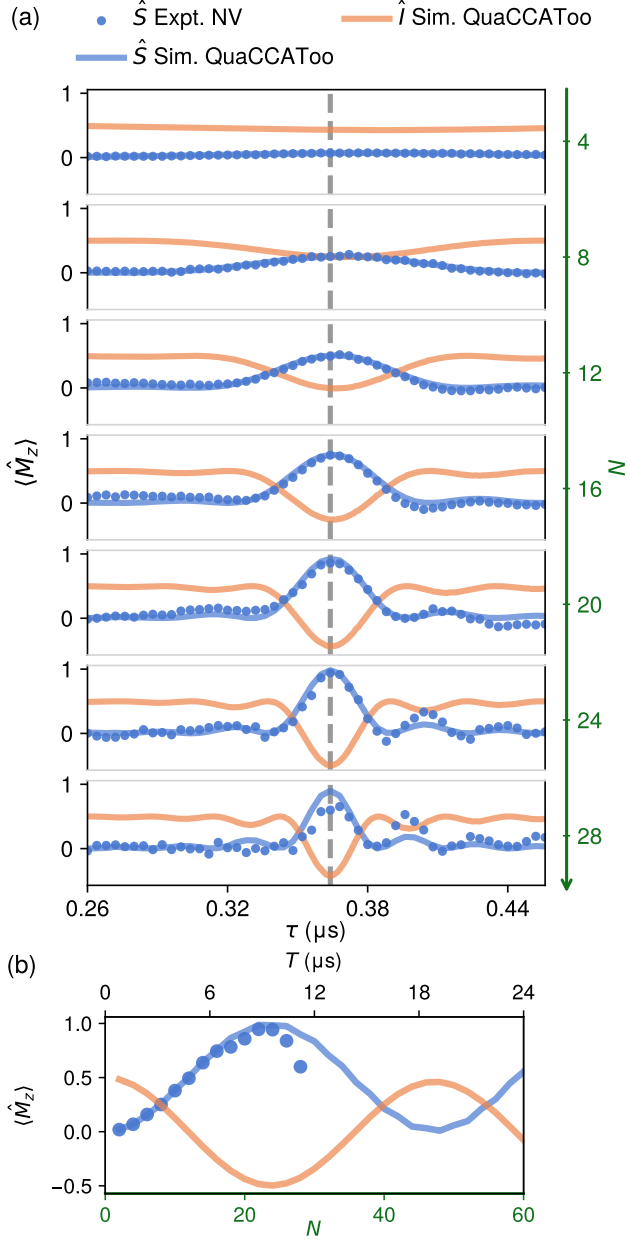


FIG. 7. (a) XYN spectrum from ^{15}NV . A small misalignment of $\mathbf{B}_0$ causes the precession of the ^{15}N nuclear spin to be sensed by the electron spin observable $\langle \hat{S}_z \rangle$, experimentally measured and simulated. While the experimental measurement of the $\langle \hat{I}_z \rangle$ observable was not possible in this work, its simulations indicate resonances opposite to $\langle \hat{S}_z \rangle$. As N increases, the experimental data starts to deviate from the simulations, due to decoherence and pulse errors [37]. (b) DD-gate with ^{15}NV . By taking $\tau = 0.364 \mu\text{s}$ fixed and varying N , we observe the Rabi-like oscillations of the two observables. With 24 pulses, a complete inversion of the population is observed. This corresponds to a total duration of $T_\pi = 9.04 \mu\text{s}$, which can represent a speed up of nearly 10 times compared to the direct excitation of the ^{15}N nuclear spin.

discussed in Sec. II C. Furthermore, the coherence of NV centers can also be extended by optimizing its fabrication methods [67, 68]. Independent of the sequence or system, QuaCCAToo [34] provides the means for users to simulate these DD gates to arbitrary color centers.

The simulations of the nuclear spin observable indicate that the target qubit is subject to a time-evolution opposite to the central spin, as seen in Sec. II with the IBMQ model. With $T_\pi = 9.04 \mu\text{s}$, we also observe a full population inversion of the nuclear spin populations with pseudo-fidelity $\bar{F} = 0.980$ [Fig. 7 (b)]. If instead we wanted to perform a π rotation to the nuclear spin with a resonant RF pulse, this would require roughly $t_\pi^{RF} = |\gamma^e/\gamma_n| t_\pi^{MW} = 83.4 \mu\text{s}$, assuming the same driving field intensity for the MW and RF fields (see Appendix A 2). Therefore, this DD-gate has the potential to not only achieve fidelities close to 1, but also to speed up the nuclear gates by nearly 10 times. Still, the simulations of the nuclear spin observable are open to experimental verification.

C. Polarization Generation for Mixed Initial States

A valuable application of this DD-gate is for the polarization of the coupled qubits. At room temperature and the typically employed magnetic fields with intensities in the orders of a few mT up to hundreds of mT, the nuclear spins coupled to the NV are nearly in a maximally mixed state. Where this thermal polarization given by the Boltzmann distribution is not enough for many quantum technology protocols, differently from nuclear magnetic and electron paramagnetic resonances. Therefore, a solution which is able to polarize the spins coupled to the NV is highly valued. Different methods have been developed for polarization of spin ensembles [69, 70] and the ^{15}N nucleus [35] coupled to the NV. But here, we propose a new method with less restrictive experimental constraints, based on simple dynamical decoupling sequences, without requiring RF pulses to nuclear spin, precise magnetic field alignment, intricate pulse generation or long coherence NV diamond samples.

The pulse error resilience analysis performed in Sec. II C indicates that the CPMG and XYN give rise to fundamentally different resonant responses from the target qubit. Yet, they also behave differently depending on the initial state of the target qubit. To show that, Fig. 8 (a) presents simulations of the NV spectrum under CPMG and XYN sequences considering an initial state $|0\rangle\langle 0| \otimes \hat{\mathbb{1}}/2$. The number of pulses N is varied, while considering the same experimental parameters as in Sec. III B, apart from the initial state. Firstly, the electronic spin under the XYN sequence gives the same resonances as observed in Fig. 7 (a) when considering the initial state $|m_S = 0\rangle \otimes |m_I = +1/2\rangle$. This shows that $\langle \hat{S}_z \rangle$ is indifferent to the initial state of the nuclear spin in the XYN sequence. By comparing the central spin resonance between the two sequences, we also observe that XYN generates narrower linewidths and

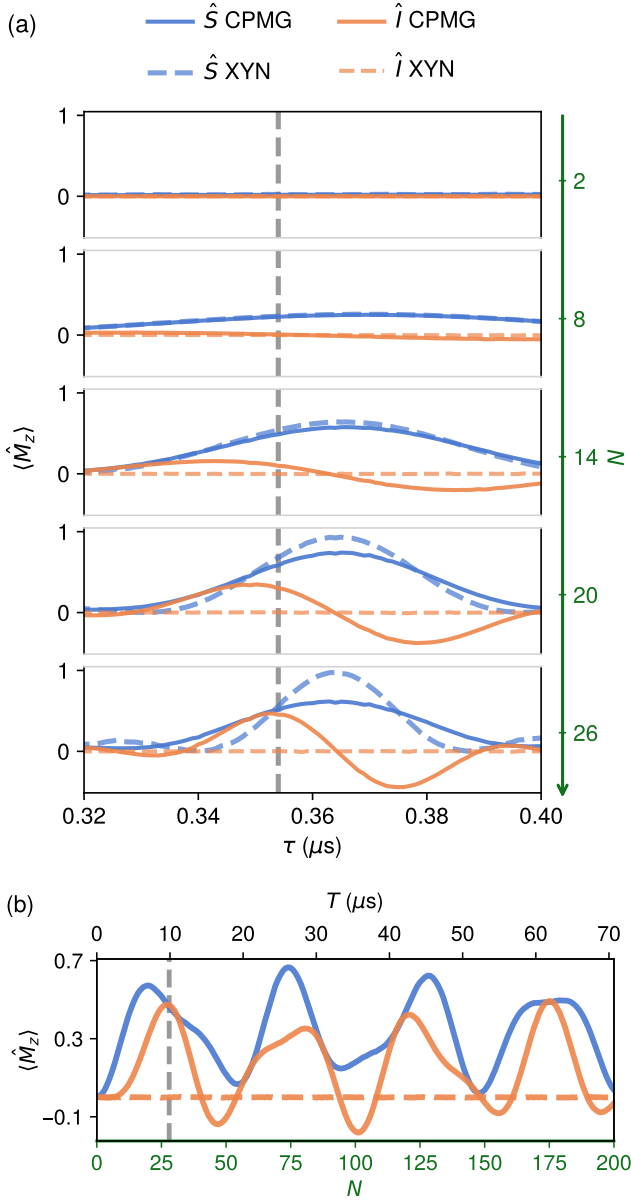


FIG. 8. (a) Simulated ^{15}NV observables under CPMG and XYN sequences for different number of pulses N , with an initial state $\hat{\rho}_0 = |0\rangle\langle 0| \otimes |\hat{1}/2\rangle$. In the XYN sequence, $\langle \hat{S}_z \rangle$ is invariant with the initial state of the target qubit, while $\langle \hat{I}_z \rangle$ remains constant. Contrastingly, the CPMG sequence induces a completely different dynamics to the initially mixed nuclear state, showing an antisymmetrical resonance around $\tau = 0.364 \mu\text{s}$. (b) Simulated polarization generation of the target qubit by DD-gate. By keeping $\tau = 0.3534 \mu\text{s}$ fixed and varying N , the two observables perform anharmonic oscillations of their expectation values. Where with $N = 27$ pulses totaling $T_{\text{pol}} = 9.54 \mu\text{s}$, $\langle \hat{I}_z \rangle$ reaches its maximum value corresponding to a polarization efficiency of 0.950, while the electron $\langle \hat{S}_z \rangle$ is perfectly mixed. This way, the initial polarization of the electron spin is transferred to the nuclei, mediated through entanglement terms.

more intense resonance peaks than CPMG.

The most prominent difference between the two sequences, nonetheless, arises from the comparison of the coupled nuclear spin response in each sequence. In the XYN sequence, the nuclear spin observable shows no variation, maintaining a constant value of $\langle \hat{I}_z \rangle = 0$. A behavior which is somewhat intuitive for a qubit that undergoes an unitary evolution having an initial state $\hat{1}/2$. On the other hand, the CPMG induces variations in the $\langle \hat{I}_z \rangle$ observable even for an identity initial state, being 0 at the resonant τ and anti-symmetrical around this point. This is not violating the unitarity of the time-evolution, because as shown in Fig. 3 (a) and discussed in detail in Sec. II B, the DD sequence is able to alter the Bloch sphere radius (the mixing) of the coupled qubit subsystem, obtained from a partial trace of the whole system (Eq. 7). Reversely to what is performed with IBMQ, it is then possible to obtain a polarized state from an initially mixed one.

To further characterize this effect of polarization generation of the coupled spin, we show the simulated time evolutions of both observables in the CPMG sequence for fixed pulse separation $\tau = 0.3534 \mu\text{s}$ and varying N . For comparison, we also show the nuclear spin observable in the XYN, which remains nearly constant even for a large number of pulses. Both observables in the CPMG perform anharmonic oscillations, which also continue indefinitely without pulse errors, decoherence or relaxation. By taking $N = 27$ with $T_{\text{pol}} = 9.54 \mu\text{s}$ in the CPMG sequence, we have a maximum of the $\langle \hat{I}_z \rangle$ observable during the oscillation, corresponding to $\langle \hat{I}_z \rangle = 0.475$. Hence, representing an efficiency of 0.950 compared to the maximum possible value of $\langle \hat{I}_z \rangle = 0.5$. At this value of τ , the electronic observable is also close to 0.5, half of its maximum value of 1.

In order to demonstrate that the final state of the nuclear spin is actually polarized, we simulate a quantum state tomography, as shown at the Appendix in Fig. 10. This demonstrates that the final state is $\hat{1}/2 \otimes |m_I = +1/2\rangle\langle m_I = +1/2|$, with a fidelity of 0.979. The fact that the electron ends the DD-gate in a mixed state evidences an interesting phenomenon, where its initial polarization is transferred to the coupled qubit. If we instead take the anti symmetrical τ point above the resonance where $\langle \hat{I}_z \rangle$ is negative, we are able to polarize the nuclear spin into the other state. Altogether, this demonstrates the possibility for a high-fidelity polarization generation through a simple CPMG sequence of the NV central spin. Clearly, this prediction also requires future experimental validation.

IV. CONCLUSION AND OUTLOOK

The ability to perform robust, high-fidelity multi-qubit gates is a cornerstone of quantum information processing. In this work, we provide a general framework for the implementation of such multi-qubit gates through DD of a central qubit coupled to target qubits. The critical

role of DD is underscored, enabling precise, fast and high-fidelity control of the target qubits, by mitigating environmental noises and eliminating the need for long, error-prone resonant control of the target qubits. The DD-mediated gates are thoroughly analyzed and cross-platform implemented with IBMQ and NVs, supported by numerical simulations within the two different frameworks

Initially, we propose and develop a general model with minimal hardware assumptions (Sec. II). Where the non-adoption of rotating frames and other perturbative approximations [41, 63] to the time-evolution of the system enables the model to operate with arbitrary couplings, which do not commute with the rotation operators for the rotating frame. Furthermore, the static laboratory solution of the qubits dynamics is able to straightforwardly incorporate pulse errors within the control field (Sec. II C).

This minimal model for DD-gates is comprehensively benchmarked within a general-purpose digital quantum simulator, represented by the IBMQ. Where the experimental realization of the DD-gates combined with Qiskit simulations [32] of the superconducting hardware reveal an interesting quantum mechanical dynamics at play. The presence of a coupling between control and target qubits gives rise to resonances in the DD spectrum (Sec. II B), which can be leveraged to obtain state transitions of the target qubit without its direct control by direct excitation. Upon further analysis of the time-evolution, we observe that the DD-gate does not correspond to proper qubit rotations. Instead, the qubits evolve from one state to another through points inside the Bloch sphere, mediated through entanglement terms of the full system density matrix.

While we experimentally demonstrate near unity fidelities for the two-qubit DD-gates with IBMQ, the implementation with three-qubit gates result in lower values (Sec. II D). This expressive reduction in performance does not indicate a limitation of the DD-gate method itself, but rather a more fundamental challenge within current noisy intermediate-scale quantum (NISQ)-era [71] hardware. That is, to emulate a time-dependent Hamiltonian in a digital gate-based architecture, as provided by IBMQ. This underscores the necessity for specialized analog quantum simulators [72], in which time-dependent Hamiltonians can be physically implemented in a direct way. Thereby avoiding errors introduced by Trotterization [73] and compilations.

The strong agreement between the theoretical model and IBMQ experimental data demonstrate the hardware-agnosticism of the DD-gate method. Thus having the potential for being employed with other systems, which are fitting with the central-target qubits description. Notably, our gate method is shown to be particularly well-suited for color centers. Where we extend the minimal model to an experimentally realistic case with ^{15}NV centers in diamond (Sec. III A), numerically simulated with the QuACCAToo software. The electronic spin of the center is used as the control qubit to induce the DD-gate

into the ^{15}N nuclear spin. In which the experimental measurements of the electronic spin and simulations of the nuclear indicate the possibility of high-fidelity control of the target qubit, with substantial speedups in gate duration as compared to direct excitation or previous DD-mediated methods [38]. The experimental implementation with NVs also highlights the sensitivity of the protocol to pulse imperfections, where at longer pulse sequences we observe discrepancies with the simulation model. These errors have the potential of being significantly mitigated by employing advanced pulse sequence engineering techniques [51–55].

Another possible application of the DD-gates is for the generation of polarization of the target qubits, which are commonly in initially mixed thermal states. Here, we propose and simulate a high-efficiency method with NVs using a simple CPMG sequence. This could represent a significant simplification of the experimental conditions of current methods for polarization generation, by not requiring precise magnetic field alignment [35] or intricate pulse sequences [69, 70]. The natural progression of this work is then the experimental verification of the proposed polarization protocol. In addition to the measurement of the ^{15}NV nuclear spin observable (Sec. III B), in order to fully validate the DD-gate application with NVs.

Further generalizations of the model can be obtained by introducing interactions between the target qubits, which are in good approximation neglected in this work. But could potentially be leveraged by the DD technique as well, in order to obtain even more robust multi-qubit DD-gates. This study also focused on only two possible initial states for the target qubit: $|0\rangle$ and $\hat{1}/2$, representing a part of a broader operational landscape. Moreover, the intermediate values for the number of pulses N between the initialization of the pulse sequence and the complete population inversion of the target qubit can potentially be employed for the generation of deterministic entangled states with high concurrence (Sec. II B). An effect which is not analyzed in depth in this work. Future studies can then characterize the complete quantum channel induced by the DD-gates, enabling its utilization in general quantum algorithm applications.

Finally, this work provides a critical step towards practical quantum technology implementations with NVs. Scalability is paramount for applications such as the diamond-based quantum token [9, 28], which requires identical operation across different NVs. Thereby using the intrinsic ^{15}N spin instead of stochastic ^{13}C nuclei as in previous studies [21–26], we transition from a system where the interactions are limited by random lattice positions to a deterministic interaction. This shift from a stochastic to a deterministic system is essential for technological scalability of future quantum devices.

DATA AND CODE AVAILABILITY

Simulations regarding NVs are open source and can be found at the QuaCCAToo documentation [34], while the simulations and experimental implementation with IBMQ are provided in the author’s Github repository [36]. The experimental data used in this work is available for scientific use upon reasonable request.

AUTHOR CONTRIBUTIONS

L.T. conceptualized this work, developed the theory, performed experiments and simulations with IBMQ and NV center. M.D. assisted in the experiments with NV center. K.V. developed and maintained the experimental setup for the experiments with NV center, and participated in the development of QuaCCAToo. B.N. acquired funding and supervised the work. All authors contributed to the writing of the text.

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Appendix A: Experimental and Simulation Methods

1. IBMQ and Qiskit

All experiments with IBMQ were performed within the Qiskit software development kit [32] version 2.1.0 and executed in the Torino quantum processing unit via Qiskit Runtime architecture version 0.40.1. The simulations of IBMQ with realistic noise models were executed locally with Qiskit Aer simulator version 0.17.1. Given the fast development of the Qiskit software ecosystem, the codes provided at [36] and used in this work may be outdated. The Hamiltonians (Eqs. 2 and 3) are constructed based on the sparse Pauli operators representation from Qiskit. Which are then used to create the time-evolution

operators (Eqs. 4 and 5) with Pauli evolution gates, synthesized via Lie Trotterization with one repetition [73]. Each Pauli evolution gate is appended to the quantum circuit respecting time-ordering, with discretized times during pulses (Sec. II A). The measurements were run with 100 shots, except for the Bloch sphere tomography in Fig 3 (a), which was run with 500 shots for a better state reconstruction.

For transpilation of the high-level representation of the circuits to the native hardware gates, we use an optimization level 2, with inverse cancellation of gates but not commutative cancellations. The dense layout method is used, taking the qubits with longest coherence and smallest gate times. Lastly, for translation, the gates are synthesized without any approximation. The transpiled circuits are then added with the mapped observables to the primitive unified blocs list and experimentally executed in the IBMQ or simulated with Aer. All experiments in IBMQ Torino were executed between July and August 2025, with minor fluctuations in some of the hardware parameters, as evidenced by the calibration reports. In any case, this does not affect the results here presented.

2. NV and QuaCCAToo

The NV center used in this work was fabricated in an electronic grade diamond plate (Element Six UK Ltd.) via ^{15}N ion implantation with energies between of 20–30 keV and dose of 10^9 $^{15}\text{N}/\text{cm}^2$. The experimental measurements with the NV center were performed on a custom-built confocal microscope, as described in detail in Refs. [37, 74]. In short, the external magnetic field $|\mathbf{B}_0|$ is applied using a permanent magnet, with four degrees of freedom. The misalignment angle and field intensity are obtained from fits of the optically detected magnetic resonance spectrum [75]. The NVs are initialized and measured with a diode laser of wavelength 518 nm, focused on the NV with an air objective. The photons are then detected and counted, giving the fluorescence observable. MW pulses for the central spin control are generated by an arbitrary waveform generator, which are then amplified and transmitted to the diamond through a thin copper wire ($d \approx 20$ μm), resulting in a π -pulse duration of $t_{\pi}^{MW} = 12.85$ ns, determined from Rabi oscillations [39]. For this value of pulse-duration, the energy difference between the $m_S = \pm 1$ levels is much larger than the bandwidth of the pulse and the system can be well approximated as a two-level system, even though QuaCCAToo simulations do not rely on this approximation. $\pi/2$ -pulses are included before and after the sequence to rotate the electron spin from and to the quantization axis, or in the case that the number of pulse blocks $N/2$ is odd, the final pulse is $3\pi/2$ to preserve the sign of $\langle \hat{S}_z \rangle$. All experimental control and data acquisition are done through the Qudi software [76].

QuaCCAToo version 1.1.0 was used to simulate the NV dynamics in the DD-gates. The NV and XY pre-defined

classes are used to model the NV systems and the XYN sequence respectively, with the same parameters as experimentally measured. The experimental data processing is done through the ExpData class, where a baseline correction of order two is applied to all XYN spectra, as shown in [34].

Appendix B: Coupling Factor

An important quantity which determines the resonant response of the central and target qubits is the coupling factor A_{zx} . To characterize its effect on the DD-gates, we consider the same experimental conditions for the IBMQ as in Sec. II B, with a Hamiltonian equal to Eq. 6, but with varying A_{zx} between 0.05 to 0.35 [time^{-1}]. In this range of coupling factors, the relation $\omega_{0,0} \gg A_{zx}$ is still valid, meaning that the driving of the qubit is well-defined and harmonic. With that, the CPMG-10 sequence was experimentally measured and simulated, as presented in Fig. 9 (a). As the coupling factor increases, the resonance amplitude varies and the sidebands also get more pronounced, as similarly observed when N is changed [Fig. 2 (a)]. We again observe strong agreement between experiment and the simulation model.

The relation between A_{zx} and the time required for a full population inversion of the target qubit T_π is particularly interesting for the experimental design of the DD-gates. As well as the resulting pseudo-fidelity of the gate $\tilde{F}$. To obtain these values, we simulate the CPMG sequences with fixed $\tau = 0.5$ [time] and different number of pulses N . This leads to a series of Rabi-like oscillations as in Fig. 2 (b), which we fit with trigonometric functions, thus obtaining the T_π and $\tilde{F}$ values as a function of A_{zx} . Fig. 9 (b) shows that the frequency of the DD-gates is linearly proportional to the coupling factor $T_\pi^{-1} \propto A_{zx}$, following the relation $T_\pi \cong 0.212/A_{zx}$ for these Hamiltonian parameters. However, it is important to note that T_π is also influenced by other factors, such as the Larmor frequency of the target qubit.

It is clearly advantageous to have a strong coupling term for having short gates, but on the other hand, the fast driving of the target qubit results in a lower pseudo-fidelity $\tilde{F}$ for a full population inversion, as indicated in Fig. 9 (c). At very weak couplings around $A_{zx} = 0.1$ [time^{-1}], the pseudo-fidelity reaches values close to 1, which then decays non-linearly to below 0.7 at $A_{zx} = 1$ [time^{-1}]. This can be attributed to the discretized nature of the pulse number variable N , that with a faster oscillation is less likely to correctly determine the exact point in time of the full population inversion of the target qubit.

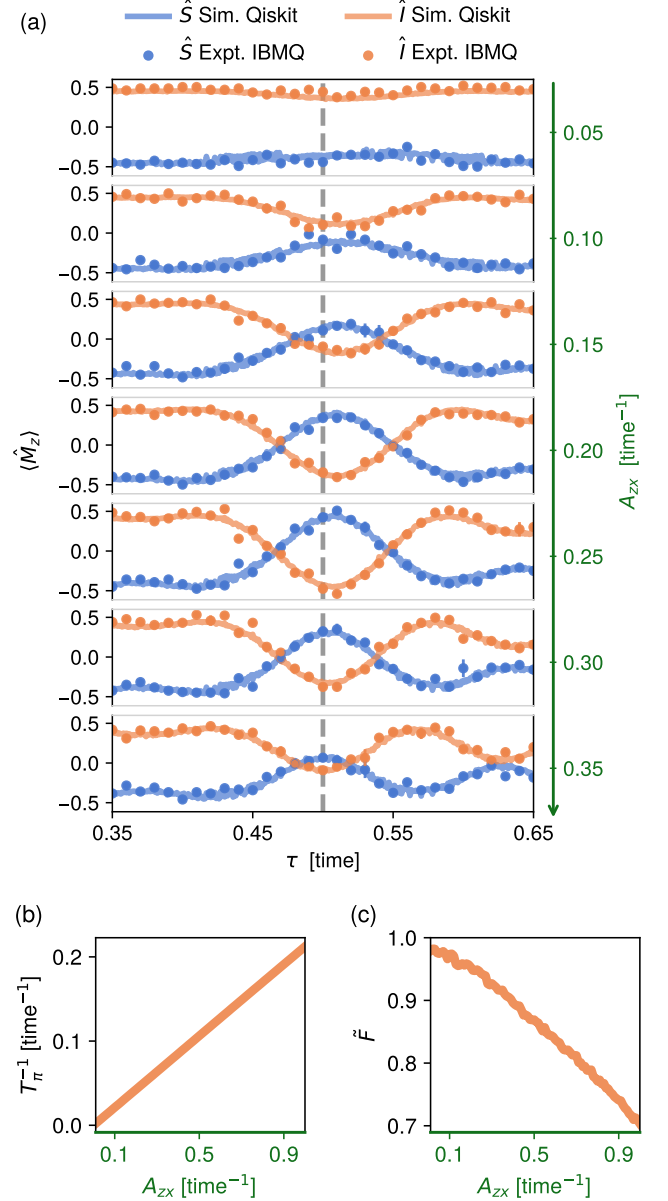


FIG. 9. (a) Experimental and simulated CPMG-10 sequences in IBMQ for different values of coupling factor A_{zx} . As A_{zx} increases, the resonance amplitude changes and the sidebands become more pronounced. (b) Simulated frequency of the DD-gate T_π^{-1} as a function of A_{zx} . T_π^{-1} is linearly proportional to A_{zx} , showing that the DD-gate becomes faster with the coupling factor. (c) Simulated pseudo-fidelity of the DD-gate $\tilde{F}$ as a function of A_{zx} . $\tilde{F}$ experiences a non-linear decrease with A_{zx} , as with a faster DD-gate, the discrete pulse number parameter N is less likely to determine the exact time for the population inversion of the target qubit.

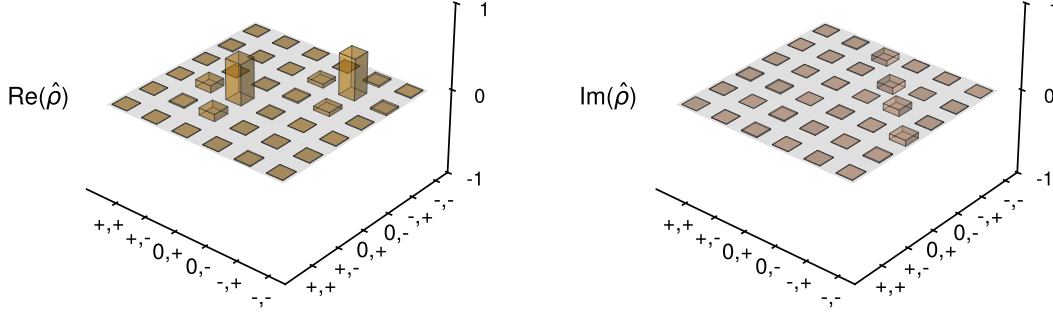


FIG. 10. Simulated quantum state tomography of the polarization generation DD-gate applied to ^{15}NV (Sec. III C). By applying a CPMG-27 sequence totaling $9.54\ \mu\text{s}$ to an initial state $\hat{\rho}_0 = |0\rangle\langle 0| \otimes |\hat{1}/2\rangle$, the initial polarization of the electronic spin is transferred to the ^{15}N nuclear spin, with a fidelity of 0.979 in relation to the state $|\hat{1}/2\rangle \otimes |m_I = +1/2\rangle$ ($|m_I = +1/2\rangle$). This method for polarization generation to the target qubit can represent a significant simplification in the experimental design of present techniques [35]. The states are labeled as $|\pm, \pm\rangle \equiv |m_S = \pm 1\rangle \otimes |m_I = \pm 1/2\rangle$ and $|0, \pm\rangle \equiv |m_S = 0\rangle \otimes |m_I = \pm 1/2\rangle$.

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