

Efficiency of optimal control for noisy spin qubits in diamond

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Decoherence is a major challenge for quantum technologies, whose negative effects can be mitigated by quantum optimal control. The decoherence dynamics significantly varies depending on the characteristics of the system's environment, consequently affecting the optimization outcomes. In this work, we investigate the optimization of a negatively charged nitrogen-vacancy (NV^-) center qubit-spin-inversion control pulse, and observe two error-compensation mechanisms, depending on how long the correlation time is compared to the pulse duration. Additionally, we analyze the effects of control space constraints and optimization options to identify a strategy to improve the optimization performance. Finally, we present experimental realizations of the optimized pulses, exhibiting the applicability of the procedure. Our work serves as a generic yet essential guide to implementing optimal control in the presence of realistic noise.

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I. INTRODUCTION

The potential applications of quantum systems for practical, scalable technologies are hindered by their inevitable interaction with the environment, leading to the loss of quantumness known as *decoherence*. A prominent example is a negatively charged nitrogen-vacancy (NV^-) center in diamond, herein referred simply as *the NV center*. The NV center is known for its long coherence time at room temperature and broad applications in quantum sensing [1–9], quantum computing [10,11], quantum networks [12,13], electric-field sensing [14], electrochemical sensing [15], magnetic imaging [16,17], magnetic resonance spectroscopy [18], masers [19,20], relaxometry [21,22], gyroscopy [23], single-photon source [24], fluorescent biomarkers, thermometry [25], biosensing [26], and magnetic biomedical applications [27], supported by accessible synthesis methods such as chemical vapor deposition (CVD) [1,3]. Despite its wide applicability, it suffers from decoherence due to interactions with the surrounding spin bath.

An NV quantum bit (qubit) can be established by isolating two out of the three ground-state energy levels of the spin-1 NV center using a static magnetic field [1,2]. Decoherence in the system [28] affects the fidelity of pulses used for coherent control via Rabi oscillation, e.g., for dynamical decoupling (DD) sequences that suppress the effects of decoherence [29–34]. The control fidelity can be improved by applying the pulse as fast as possible, but this is not generally viable due to practical limitations, e.g., in pulse power. More practical strategies are developed for robust qubit control, including composite pulses [35–42], continuous driving [31,43–49], rapid adiabatic passage [30,50–57], stimulated Raman adiabatic passage [58–62], shortcuts to adiabaticity [63–66], and quantum optimal control [1,67–72].

This work concerns quantum optimal control (QOC), which uses iterative algorithms to optimize the control pulse based on the control's degrees of freedom. Distinctively, QOC methods do not require additional mechanisms, such as pulse dressing, which may introduce additional constraints to the system and require a deeper analysis. The versatility of QOC makes it highly applicable and adaptable to a wide range of control problems, such as in quantum sensing [1,73,74], quantum information processing [1,75–79], and dynamical decoupling [73,77,78,80]. Furthermore, it complements other strategies to provide robust operational performance [60,76,81].

The properties of the NV center, e.g., its coherence time, vary depending on its environment [82–85], leading

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us to question how QOC optimization results vary with the environmental noise. The Ornstein-Uhlenbeck (OU) process [86–88] has been widely used for describing decoherence in NV centers in diamond, and its applicability has been confirmed experimentally [4,9,30–32,48]. Apart from NV centers, the model has also been directly applied to other quantum systems, e.g., germanium vacancy centers in diamond [89,90] and trapped ions [91]. Despite the widespread usage of the OU process to model decoherence, there has been no dedicated study so far investigating how the environmental noise parameters, e.g., correlation time, affect the optimization outcome. Specifically, the optimized pulse is found to differ when it is built for different time windows [60,76], and when the optimization algorithm parameters and goal vary [75,78]. This motivates us to study and analyze how the parameters of the qubit environment affect the resulting optimized dynamics. While the study is focused on NV centers, it is also applicable to other physical systems where QOC methods are applied to optimize qubit dynamics, e.g., in superconducting qubits and trapped ions.

Our work presents a guideline for optimal control of a qubit under two nonideal cases: environment-induced decoherence and control amplitude noise. We build a control landscape appropriate for the given problem and use a commonly used optimal control scheme, namely the dressed chopped random basis (dCRAB) [92] with the Fourier basis option, to optimize the control pulse for spin inversion under decoherence dynamics represented by OU noise processes with different environment-noise correlation times. We find that the optimized pulse shape depends on the noise correlation time is longer than the pulse duration. Longer correlation times result in pulses that temporarily backtracks the qubit operation to compensate for the noise effects, while shorter correlation times result in pulses that are squeezed to the maximum allowable amplitude to complete the operation within the shortest period possible. In addition, we analyze how various optimization options affect the optimization outcomes. By appropriately relaxing the constraint on the spatial components of the optimized pulse, as well as increasing the number of scheme-specific variables, we observe significant changes in the pulse shape, albeit an overall worse performance for the given computational expense due to the increased control space complexity. We then allow more wiggle features during the optimization, and observe improved pulse performance for low correlation times, showing that the feature is beneficial in that case. Finally, we experimentally generate selected optimized pulses and compare it to the numerical results. The good agreement in pulse shape and performance between them showcases the feasibility of the optimization procedure in an experimental setting.

The remainder of this paper is organized as follows. In Sec. II, we describe the system dynamics starting from the qubit description for an NV center, then introduce

the nonidealities and visualize how different decoherence dynamics are obtained by varying the parameters from their mathematical descriptions. Section III describes the control problem, objective, constraints, and QOC scheme used (i.e., the dCRAB algorithm). Section IV presents and discusses the optimization results, namely the variation of the pulse’s general feature with the decoherence dynamics, the effects of the optimization options, and the experimental feasibility of the procedure. We discuss challenges and provide outlooks in Sec. V, and finally conclude our work with Sec. VI.

II. SYSTEM AND NOISE PROCESSES

A. The ideal nitrogen-vacancy qubit Hamiltonian

The NV center is a spin $S = 1$ system. In the absence of an external magnetic field, the ground $m_s = 0$ and degenerate $m_s = \pm 1$ energy levels are separated by $E_{\text{zf}} \approx h \times 2.87$ GHz, where h is Planck’s constant and zf stands for “zero field”. Under a static magnetic field $\vec{B}_0$ of magnitude B_0 , the $m_s = \pm 1$ levels undergo the Zeeman splitting [93]. Taking the $m_s = 0$ level to be the zero of energy, the three levels are described mathematically by

$$E(m_s) = |m_s|E_{\text{zf}} + \hbar m_s \gamma B_0, \quad (1)$$

where $\hbar = h/2\pi$ and $\gamma \approx 2\pi \times 28$ MHz/mT is the gyro-magnetic ratio. The NV center can be reliably initialized in the $m_s = 0$ state by using optical spin pumping [1,2,93].

An NV qubit can be established by using a sufficiently large B_0 to isolate two of the three ground-state levels, including the $m_s = 0$ state. Using control pulses resonant with the transition frequency between the two states, the transitions involving the third energy level become practically negligible. This allows us to work in a two-level Hilbert subspace of the system, approximating it as a qubit. Mathematically, the qubit approximation can be done via adiabatic elimination (see, e.g., Ref. [94]). Here, we follow a more heuristic approach and write down the widely used qubit Hamiltonian to represent the NV qubit (see, e.g., Ref. [49]). Setting $\hbar = 1$ herein, it is given by

$$\hat{H}_S(t) = \frac{\omega_0}{2} \hat{\sigma}_z + \Omega_1 f(t) \cos[\omega_0 t + \phi(t)] \hat{\sigma}_x \quad (2)$$

in the Schrödinger picture. Here, the Larmor frequency ω_0 corresponds to the energy splitting between the two levels making up the qubit, denoted $|0\rangle = (0 \ 1)^T$ and $|1\rangle = (1 \ 0)^T$ for the lower and upper state, respectively. Qubit control is achieved using a linearly polarized oscillating magnetic pulse $\vec{B}_1 = B_1 f(t) \cos[\omega_0 t + \phi(t)] \hat{x}$ applied in the plane perpendicular to $\vec{B}_0$. The time-dependent functions $f(t)$ and $\phi(t)$, respectively, amplitude and phase modulate the control pulse. As a result, the base Rabi frequency $\Omega_1 = \gamma B_1 / \sqrt{2}$ is modulated by $f(t)$. The pulse

frequency ω is ideally tuned to be resonant with the qubit transition frequency, i.e., $\omega = \omega_0$ so that a total population inversion is possible (see Appendix A). We also require that $\Omega_1 \ll \omega_0$ to avoid strong-driving effects, such as the Bloch-Siegert shift [95,96]. In the Bloch-sphere representation in the Schrödinger picture, Rabi oscillation is represented by a spiraling motion as the Bloch vector of the qubit moves up and down the sphere's surface due to the driving field.

It is worth noting that coherent interactions with proximal nuclear spins can be significant to the system's dynamics, but are ignored in this model. However, under a strong enough driving field, the effects of such interactions can be considered a moderate, effective detuning of the NV electron-spin-transition frequency, which can be effectively refocused by robust pulses and dynamical decoupling [9,89], the former being the goal of this work.

A simpler dynamics can be observed by moving into the interaction picture with respect to $\hat{U} = \exp(i\omega_0 \hat{\sigma}_z t/2)$, which implies that the interaction picture is a frame rotating at the Larmor frequency of the qubit. Applying the rotating-wave approximation (RWA) [50], where we assume that $\Omega_1 f(t) \ll \omega_0$, we obtain

$$\begin{aligned} \hat{H}_I(t) &= \hat{U} \hat{H}_S \hat{U}^\dagger - i\hat{U} \frac{d\hat{U}^\dagger}{dt} \\ &\approx \frac{\Omega_1}{2} f(t) \{ \cos[\phi(t)] \hat{\sigma}_x + \sin[\phi(t)] \hat{\sigma}_y \}. \end{aligned} \quad (3)$$

The RWA assumption is feasible as ω_0 is typically of order of GHz for NV centers in diamond and $\Omega_1 f(t)$ is usually in the range of tens of MHz [93]. In the interaction picture, the Rabi oscillation is represented as a motion along the longitude of the Bloch sphere without the rotation along the latitude. The RWA approximates the exact dynamics better as the rotation frequency of the rotating frame gets larger [97].

Throughout this work, we set $\Omega_1 = 2\pi \times 1$ MHz for convenience and limit $|f(t)| \leq 5$, so that the control parameters are applicable for most experiments with NV centers in diamond [93]. We also allow $\Omega_1 f(t)$ to be negative. A rotation with frequency $\Omega_1 f(t) < 0$ about an axis represented by ϕ is equivalent to a rotation with frequency $|\Omega_1 f(t)|$ about the axis represented by $(\phi + \pi) \bmod(2\pi)$. In the Bloch-sphere representation, a clockwise rotation about the former axis and a counterclockwise rotation about the latter axis are the same operation.

B. Nonidealities with Ornstein-Uhlenbeck processes

The NV qubit is subject to magnetic noise via magnetic dipolar interactions with the surrounding N spins. The random flips of the surrounding spins result in noisy shifts of the qubit's Larmor frequency, causing dephasing. The resulting dynamics is a coherence decay, as measurable using the Ramsey measurement scheme [28,82,83,

98]. We mathematically model this nonideality using a fully relaxed Ornstein-Uhlenbeck (OU) process [99–101], which can be numerically generated using the following updating formula:

$$X(t + \Delta t) = X(t)e^{-(\Delta t)/\tau} + \tilde{n}\sqrt{\frac{c\tau}{2}}(1 - e^{-2(\Delta t)/\tau}), \quad (4)$$

which is exact for an arbitrary Δt . The initial value $X(0)$ is randomly sampled from a Gaussian distribution with mean 0 and variance $c\tau/2$, while $\tilde{n}$ is sampled from a standard Gaussian distribution. The quantities c and τ are the OU parameters called the diffusion constant and the relaxation time, respectively. The fully relaxed OU process has the property that at any given time t , the process $X(t)$ is Gaussian distributed with a constant mean of 0 and variance of $\sigma^2 = c\tau/2$. Since c only appears in Eq. (4) as σ , we use σ and τ as the OU parameters henceforth. Using σ is useful as it contains the information about the variance of $X(t)$ at any given time.

We denote the effect of magnetic noise on the detuning of the NV qubit as $\delta(t)$ and call it “the δ noise” herein. This model is convenient due to the straightforward correspondence between the OU parameters and experimental data [4,9,30–32,48,89–91]. The coherence time T_2 is the time it takes for the system's coherence to fall to $1/e$ of its initial value under the given evolution. Let T_2^* and T_2^{HE} be the coherence times during a Ramsey measurement and a Hahn-echo sequence, respectively. Then, the OU parameters σ_δ and τ_δ of the δ noise are obtained by measuring experimentally T_2^* and T_2^{HE} [89,90] and solving the system of equations (see Appendix B for the derivation)

$$\begin{aligned} 4\tau_\delta e^{-T_2^{\text{HE}}/2\tau_\delta} - \tau_\delta \left(e^{-T_2^{\text{HE}}/\tau_\delta} + e^{-T_2^{*}/\tau_\delta} + 2 \right) \\ + T_2^{\text{HE}} - T_2^* = 0 \end{aligned} \quad (5)$$

for τ_δ , and then by computing

$$\sigma_\delta = \left(\tau_\delta^2 e^{-T_2^{*}/\tau_\delta} - \tau_\delta^2 + \tau_\delta T_2^* \right)^{-1/2}. \quad (6)$$

These equations assume that the control pulses are instantaneous. Practically, we may use values of T_2^* and T_2^{HE} obtained from experiments where the pulses are shorter than the coherence decay times (see, for example, Ref. [28]).

In addition to the δ noise, we consider an uncertainty in the control pulse amplitude. In an experimental setup, the magnetic-field amplitude generated by the apparatus may not be exactly what is expected. We model this uncertainty, which we denote $\epsilon(t)$ and call “the ϵ noise,” as a 5% amplitude error using a fully relaxed OU process with $\tau_\epsilon = \infty$ and $\sigma_\epsilon = \sqrt{c_\epsilon \tau_\epsilon / 2} = 0.05$.

Besides inducing decoherence, the δ noise hinders the efficacy of any control pulse with a finite width; the longer

it takes a pulse to operate on the qubit, the worse its performance will be. Meanwhile, the ϵ noise causes a deviation of Rabi frequency in each evolution sample, leading to a dephasing accumulated with the rotation phase. Consequently, the effect of the ϵ noise is more apparent for pulses with large overall rotation phases. Whether the effect of the ϵ noise dominates over the effect of the δ noise on the control pulse depends on the pulse parameters and their characteristics. We discuss this in more detail in Appendix D.

Subject to both noises, $\delta(t)$ and $\epsilon(t)$, the full Hamiltonian becomes

$$\begin{aligned} \hat{H}_I(t) = & \frac{\delta(t)}{2} \hat{\sigma}_z \\ & + \frac{\Omega_1}{2} f(t) [1 + \epsilon(t)] \{ \cos[\phi(t)] \hat{\sigma}_x + \sin[\phi(t)] \hat{\sigma}_y \}, \end{aligned} \quad (7)$$

which is typically used to describe the NV qubit dynamics under decoherence and control amplitude error [30, 31, 43, 102–105]. Under this stochastic Hamiltonian, the system undergoes decoherence and evolves into a mixed quantum state. In each realization (or sample), the system evolves under a closed system equation of motion, i.e., the Schrödinger equation or, equivalently, the Liouville-von Neumann equation. The physically relevant open system dynamics is then given by the average over many noise realizations. Given a sample size N_{sample} , the observed value of, say, $\langle \sigma_z \rangle$ is given by the sample average

$$\begin{aligned} \overline{\langle \sigma_z \rangle} &= \frac{1}{N_{\text{sample}}} \sum_{j=1}^{N_{\text{sample}}} \langle \sigma_z \rangle_j \\ &= \frac{1}{N_{\text{sample}}} \sum_{j=1}^{N_{\text{sample}}} \text{tr}(\rho_j \hat{\sigma}_z), \end{aligned} \quad (8)$$

where $\rho_j(t)$ is the density matrix obtained by evolving the system with the Hamiltonian given by Eq. (7) for the j th noise realization. The overline in $\overline{\langle \sigma_z \rangle}$ denotes the average of the expectation values $\langle \sigma_z \rangle_j, j = 1, \dots, N_{\text{sample}}$ over all noise realizations. We provide a more detailed interpretation of this stochastic Hamiltonian in Appendix C.

Numerically, the sample-averaged quantities fluctuate when the calculation is repeated with different sets of OU noises due to the finite sample size. To characterize this *finite-sample statistics*, we can repeat the calculation a large number N_{rep} of times with the same N_{sample} . As N_{sample} becomes larger, the average of the distribution converges toward the true value, while the standard deviation decreases. Throughout this work, we use $N_{\text{rep}} = 100$ and $N_{\text{sample}} = 1500$, which we deem sufficient to obtain

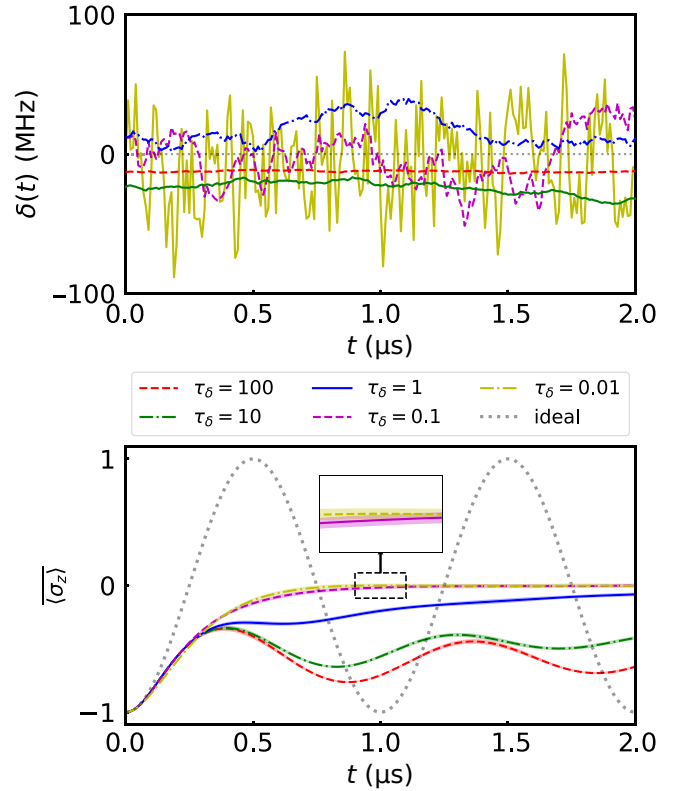


FIG. 1. Single random δ noise samples (top) and the corresponding Rabi oscillation of the sample-averaged population inversion represented by $\overline{\langle \sigma_z \rangle}$ (bottom). They are obtained by fixing the coherence decay time, $T_2^* = 0.1 \mu\text{s}$, and by varying the correlation time τ_δ of the δ noise. We consider no amplitude noise in this example simulation, i.e., $\epsilon = 0$. One Rabi period is $2\pi/\Omega_1$, where $\Omega_1 = 2\pi 1 \text{ MHz}$. The inset in the bottom figure shows small fluctuations in the average value due to the finite sample size represented by the standard deviation of the fluctuation statistics. It is obtained by repeating the simulation with different noise realizations with $N_{\text{sample}} = 1500, N_{\text{rep}} = 100$. The values for τ_δ are from Table I.

the average dynamics with sufficiently low deviations, as shown by the inset in the bottom part of Fig. 1.

C. Tuning the δ noise

The noise parameters for the NV qubit vary due to several factors, for instance, the strength of the interaction with the spin bath [82], the strength of the static field [83], the location of the NV center within the crystal, and the chemical species surrounding the center [83–85]. Therefore, it is interesting to study the dynamics of the qubit under various noise spectra. We are particularly interested in fixing the value of T_2^* and tuning τ_δ , as shown in Table I. We choose $T_2^* = 0.1 \mu\text{s}$ as an example value, which can occur in a shallow NV center situated within several nanometers under the sample surface due to unwanted interactions with surface spins [106]. The top part of Fig. 1

TABLE I. Calculated noise parameters for different δ noise spectra obtained by fixing the free evolution coherence decay time $T_2^* = 0.1 \mu\text{s}$ of the qubit and by varying the relaxation time τ_δ of the δ noise. The corresponding approximate values of the Hahn-echo coherence decay time T_2^{HE} and the standard deviation $\sigma_\delta = \sqrt{c_\delta \tau_\delta / 2}$ of the δ noise are obtained from Eqs. (5) and (6), under the assumption that the instantaneous Hahn-echo pulse does not suffer from the OU noises (see Appendix B for the detail). The corresponding noise spectra are visualized in Fig. 1.

T_2^* (μs)	τ_δ (μs)	σ_δ (MHz)	T_2^{HE} (μs)
0.1	100	2π 2.251	1.8
0.1	10	2π 2.255	0.85
0.1	1	2π 2.288	0.41
0.1	0.1	2π 2.624	0.22
0.1	0.01	2π 5.305	0.2

shows single random samples for different τ_δ values. It exhibits how the δ noise fluctuates faster in the given time window and has a more spread out distribution (larger σ_δ) as τ_δ becomes smaller.

The efficacy of a control pulse can be characterized by how long its intended operation can be effective. An example is shown in the bottom part of Fig. 1, which shows the evolution of $\langle \sigma_z \rangle$ when a constant-amplitude pulse is applied continuously over an extended period with the ϵ noise turned off. Without the δ noise, the Rabi oscillation lasts indefinitely. With the δ noise in effect, the Rabi oscillation dies out with time, with the lifetime decreasing alongside τ_δ . This, alongside the change in T_2^{HE} in Table I, shows that control pulses become less effective the smaller τ_δ gets.

III. OPTIMAL CONTROL

Here, we describe the quantum optimal control scheme used to optimize the applied pulses by introducing the control landscape description, the optimization algorithm, its options, and the initial pulses to optimize. Henceforth, the unit of τ_δ is in μs , and not explicitly written for brevity.

A. Building the control landscape

The control amplitude $f(t)$ and phase $\phi(t)$ modulation allow us to freely shape the x and y components in the system's rotating frame. They enable the control landscape for the qubit, where we can use numerical algorithms to find an optimal pulse that achieves a certain objective; this is quantum optimal control (QOC). The QOC landscape consists of system dynamics, control objectives, and control space restrictions [1]. Here, the system dynamics is given by Eq. (7), and the corresponding physical processes are thoroughly discussed in Sec. II.

The control objectives are represented by either a cost function J to be minimized or a figure of merit (FoM) to be maximized. We use the cost function J throughout

this work. Here, we are interested in how the optimized pulse shape changes with respect to the δ noise spectrum, as mentioned in Sec. II C. By understanding how the pulse behaves against various noise parameters, we may obtain insight into the optimal control pulse shape for the given noisy spin dynamics. With the NV spin qubit initially in state $|0\rangle$, we set an exemplary goal to optimize the pulse that evolves the system into state $|1\rangle$. One appropriate cost function is the sample-averaged infidelity with respect to the target state $\rho_{\text{target}} = |1\rangle\langle 1|$. While seemingly simple, a robust spin inversion is the backbone of robust, more complicated pulse sequences [107]. Given the definition of quantum state fidelity in Sec. 9.2 of Ref. [108], the cost function is given by

$$J = 1 - \frac{1}{N_{\text{sample}}} \sum_{j=1}^{N_{\text{sample}}} \text{tr} \left(\sqrt{\sqrt{\rho_j(T)} \rho_{\text{target}} \sqrt{\rho_j(T)}} \right) \\ = 1 - \frac{1}{N_{\text{sample}}} \sum_{j=1}^{N_{\text{sample}}} \sqrt{\langle 1 | \rho_j(T) | 1 \rangle}, \quad (9)$$

where $\rho_j(T)$ is the state at the end of the pulse duration T for the j th noise realization. Ideally, $\rho_j(T) = \rho_{\text{target}}$ for all j , which gives $J = 0$.

The control space restrictions bound the optimization landscape by limiting the values $f(t)$ and $\phi(t)$ may take to avoid unwanted results, such as excessive power. For our optimization, we impose the constraint

$$|f(t)| \leq 5, \quad (10)$$

which, with $\Omega_1 = 2\pi \times 1 \text{ MHz}$, bounds the Rabi frequency's magnitude under $2\pi \times 5 \text{ MHz}$, known as the “high Rabi frequency” [30].

B. dCRAB algorithm

Various optimal control schemes have been formulated and implemented. In this work, we consider the dCRAB algorithm that is commonly used for control problems involving the NV center [1,92]. One recent example is the optimization for rectifying a quantum gate-set metric experiment with an ensemble of NV centers [109]. Other than the NV center, this algorithm has been shown to succeed in optimizing various control systems, such as the Ising model [110], the dynamical Casimir effect [111], and Bose-Einstein condensates in magnetic microtraps [112].

In dCRAB, the optimization is divided into *superiterations*. In each superiteration, $f(t)$ and $\phi(t)$ are each expanded into a predetermined—not necessarily the same—number N_c of basis functions. Mathematically, we

have

$$f^s(t) = a_0^s f^{s-1}(t) + \sum_{k=1}^{N_c} a_k^s f_k^s(\beta_k^s; t), \quad (11)$$

where $s = 1, 2, 3, \dots$ and $a_0^1 = 0$. The expansion is similar for $\phi(t)$. The basis functions $f_k^s(\beta_k^s; t)$ form a complete set in the case where $N_c \rightarrow \infty$. Examples of bases to choose from include the Fourier and Chebyshev bases. Since we only use N_c basis functions, the basis is said to be *chopped*. Each basis function has a randomized parameter β_k^s , e.g., a random oscillation frequency for a Fourier basis function.

Additionally, it is customary to multiply Eq. (11) by a scaling function $\Lambda(t)$ to determine the general shape of the optimized pulse. We scale our pulse following:

$$\Lambda(t) = \tanh \left[\sigma \sin \left(\frac{\pi t}{2T} \right) \right] \tanh \left[-\sigma \sin \left(\frac{\pi(t-T)}{2T} \right) \right], \quad (12)$$

where σ determines the steepness of the scaling function as it falls toward zero at the time window boundaries. We set $\sigma = 30$ throughout this work. This ensures that the resulting pulse starts and ends at zero, making it experimentally convenient.

In the s th superiteration, the optimization looks for the optimal values of the coefficients a_0^s, a_k^s that minimize J using direct search algorithms such as the Nelder-Mead algorithm. To escape a local minimum, the optimization moves into the next super-iteration with a new set of randomized basis functions. The coefficient a_0 lets the optimization move toward the optimized pulse $f^{s-1}(t)$ obtained in the previous super-iteration. By doing this, the optimization is *dressed* with a new search direction.

C. Optimization options

One problem we address in this work is deciding on how many variables to optimize. More variables result in a larger and more complex control landscape, allowing for more possible pulse shapes. However, it becomes harder for the algorithm to find an optimum, therefore increasing the computational cost. For our control problem, this concerns whether we optimize either one of or both functions $f(t)$ and $\phi(t)$. For the dCRAB algorithm in particular, this concerns how many basis functions we use per super-iteration. To examine the trade-off between the control space and computational cost, we perform multiple rounds of optimizations with varying control landscape complexities. We progressively enlarge the control space following these cases: (1) Optimizing $f(t)$ only while fixing $\phi(t) = \pi/2$; (2) Optimizing $f(t)$ while also optimizing $\phi(t)$ as a constant; and (3) Optimizing both $f(t)$ and $\phi(t)$ as functions of time. For the latter two cases, we set $\phi(t) = \pi/2$ as the initial guess. By increasing the number of variables

this way, we progressively relax the constraint imposed on the pulse components, respectively: (1) Allowing only the y -component; (2) Allowing both the x - and y -components while constraining their shapes to be similar; (3) Allowing both components to have different shapes. Additionally, we vary the number of dCRAB basis functions N_c per super-iteration for each of the aforementioned cases. Increasing N_c allows more possible pulse shapes at the expense of a larger control space. For each of these cases, the functions $f(t)$ and $\phi(t)$ are expanded with the same N_c .

There are other optimization options in dCRAB that can affect the control landscape. One of those options is the choice of basis functions, which has been shown to significantly affect the convergence time for the optimization [113]. In this work, we only consider the conventional Fourier basis, a typical basis that has been experimentally demonstrated (see, e.g., works by [114,115]). For the Fourier basis, the randomized parameters are the frequencies of the sinusoidal components, sampled from a specified range with uniform probability. This allows us to limit the frequency component that the optimized pulse may have. Since a lower τ_δ results in the δ fluctuating faster over a given time window, we hypothesize that such noise can be counteracted by pulses with high-frequency components. For each of the above-mentioned cases, we vary the upper limit of the random Fourier basis frequency. The lower and upper limits are set to values such that the pulse period T is equal to, respectively, 0.1 and $\beta_{\max}$ times the resulting sine wave periods. Similar to N_c , we set the same $\beta_{\max}$ for both $f(t)$ and $\phi(t)$.

Optimization performances with various options are compared for the same computational resource. The numerical optimization is terminated after $N_{\text{iter}} = 2000$ total iterations to simulate a case of limited computational resource [116]. We set the same convergence condition for each superiteration: the algorithm moves into the next superiteration if J does not change by 10^{-3} on average over the last 100 iterations, which we assume to be sufficient to indicate that a local minimum has been met.

D. Pulses to optimize

The optimization algorithm requires an initial pulse. Here, we start with a rectangular pulse with amplitude $\Omega_1 = 2\pi \times 1$ MHz, with $f(t) = 1$ and $\phi(t) = \pi/2$, applied over a duration $T = 0.5$ μ s. The initial control phase is arbitrarily chosen since there is no preferred rotation axis to achieve our goal, while the pulse period is set such that it performs differently for the values of τ_δ given in Table I. With our choice of initial pulse, the optimization process may be interpreted as *letting the algorithm reshape the initial rectangular pulse*. As elaborated in Appendix D, the δ noise is dominant in this optimization problem, so our results can be explained with respect to the δ noise only. Nevertheless, we keep the ϵ noise in the simulations

and optimization runs to emphasize the generality of our approach.

Practically, it is best to use a sampling rate matching that of the waveform generator used in the experimental setup. However, to save computation time, we opt for a sampling rate that is high enough to avoid signal aliasing in all the optimization cases. This can be done by conforming to the Nyquist criterion, i.e., choosing a sampling frequency at least twice the highest-frequency component of the sampled signal. We divide our simulation window of $T = 0.5 \mu\text{s}$ into 50 time bins, each having a width of 10 ns. This translates to a sampling rate of 100 MHz, which is reliable for pulses with frequency components up to 50 MHz, corresponding to $\beta_{\text{max}} = 25$. Increasing the sampling rate does not meaningfully affect the optimization outcomes as the physical properties of the pulse are left unchanged.

IV. OPTIMIZATION RESULTS

Our optimizations are performed using the Quantum Optimal Control Suite (QuOCS) [110], a Python numerical package for QOC. We run the dCRAB algorithm using the adaptive Nelder-Mead direct search with drift compensation [117]. The package requires additional parameters to be specified. First, as $\phi(t)$ is considered a generic function of time, we set its bounds to be some large positive and negative numbers, considering its periodicity. Second, the “amplitude variation” controls how fast the variables change over the iterations. A value too large may cause the algorithm to frequently skip an optimum, while a value too small may slow the algorithm down. Here, we choose the variation to be $0.3 \times 10 = 3$ for $f(t)$ and $0.3 \times 2\pi$ for $\phi(t)$. This lets the algorithm traverse the control landscape with reasonably quick convergence toward an optimum. Finally, QuOCS provides an option to either shrink or truncate the pulse at the limits. As we are interested in the optimized pulse shape, we choose the former.

Like any other sample-averaged quantity, the cost function J fluctuates throughout the optimization runs, forming a fluctuating control landscape. Despite this seemingly unusual feature, the optimization is viable, as shown by our simulation results. We report the cost function J_{opt} for the optimized pulse using the mean and standard deviation of the finite-sample statistics discussed in Sec. II B. The standard deviations range between about 0.001 and 0.008 over all optimization cases, which are small compared to the mean values, suggesting that they are insignificant compared to the optimization scale.

The full optimization results are provided in Appendix E, which contains four figures. Figure 6 shows the optimized pulse components $f_x(t) = f(t) \cos[\phi(t)]$ and $f_y(t) = f(t) \sin[\phi(t)]$ alongside the optimized cost function values J_{opt} reported as the mean value plus-minus the standard

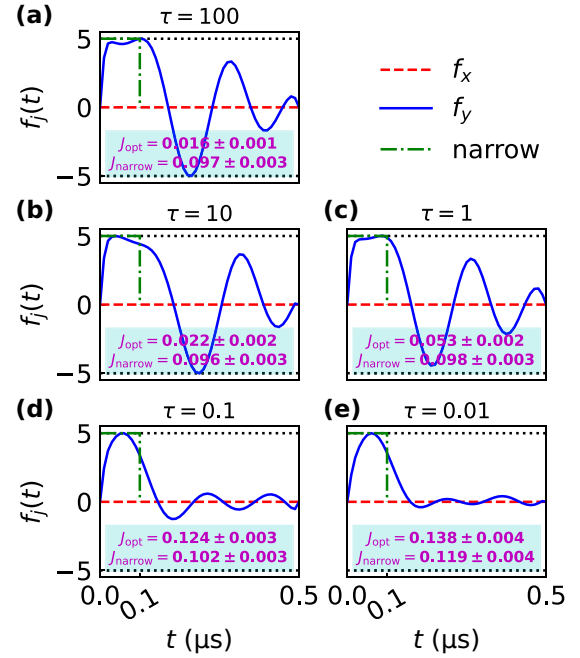


FIG. 2. Optimized modulation components $f_x(t) = f(t) \cos[\phi(t)]$ and $f_y(t) = f(t) \sin[\phi(t)]$ vs the evolution time t , for different correlation times of the noise in the detuning τ_δ . We consider the case where $f(t)$ is optimized with $\phi(t) = \pi/2$, $N_c = 5$, and $\beta_{\text{max}} = 3$ for all plots in the figure. On top of each plot, the value of τ_δ , the optimized cost function J_{opt} , and the cost function J_{narrow} for a short rectangular pulse, which we label *narrow*, are shown. The black dotted lines show the limits in the magnitude of the optimized function. The fixed parameters used here are $\Omega_1 = 2\pi \times 1 \text{ MHz}$, $N_{\text{iter}} = 2000$, $T = 0.5 \mu\text{s}$, $N_{\text{sample}} = 1500$, $N_{\text{rep}} = 100$. These figures are also located along the first row of Fig. 6 (denoted as **1.a.i.**).

deviation over N_{rep} . Additionally, we present the comparison of J_{opt} for all optimization runs in Fig. 7. The change in J over the iterations is given in Fig. 8. The evolution of $\langle \sigma_z \rangle$ with the optimized pulses are presented in Fig. 9. To aid our discussion, Figs. 2 and 3 contain optimized pulses taken from Fig. 6.

For comparison, the values of J for the initial guess are (0.559 ± 0.008) , (0.542 ± 0.008) , (0.482 ± 0.007) , (0.392 ± 0.006) , (0.378 ± 0.006) for $\tau_\delta = 100, 10, 1, 0.1, 0.01$, respectively.

A. General features of the optimized pulses

Aside from a few exceptions, our numerical simulations follow a general trend. All optimization cases improve the pulse performance, as indicated by the reported J_{opt} values, which depend on the correlation time. In most cases, J_{opt} increases monotonically as τ_δ decreases. That is, we generally have worse-performing optimized pulses as the correlation time becomes shorter, showing that the

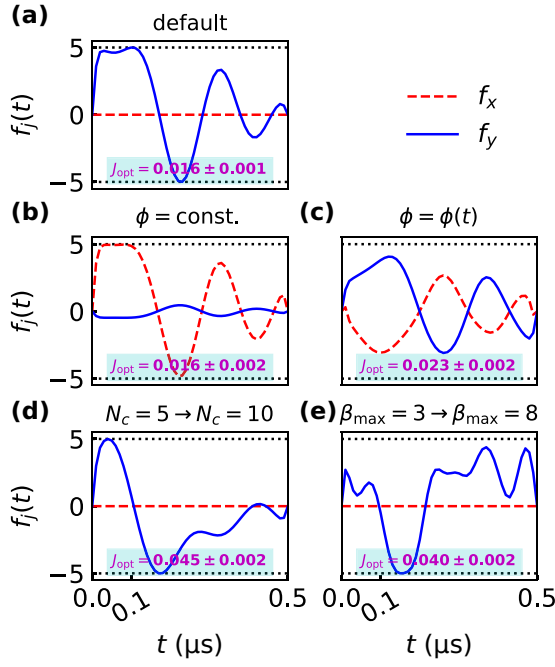


FIG. 3. Shape of the optimized pulses vs the evolution time t for correlation time $\tau_\delta = 100 \mu\text{s}$ exhibiting how the shape of the optimized pulse and the cost function change as the optimization options are modified. The optimization option parameters $[\phi(t), N_c, \beta_{\max}]$ take a set of values, as follows: (a) **1.a.i.** $[\pi/2, 5, 3]$, (b) **2.a.i.** $[\text{const.}, 5, 3]$, (c) **3.a.i.** $[\phi(t), 5, 3]$, (d) **1.b.i.** $[\pi/2, 10, 3]$, (e) **1.a.ii.** $[\pi/2, 5, 8]$. The components in (b) have the same phase relation for all t . The features of the plots are noticeably similar to Fig. 2.

noise with faster fluctuations is more difficult to counteract. We observe significantly different optimal pulse shapes, depending on whether T is shorter than the noise correlation time τ_δ , as illustrated by Fig. 2.

When $T \ll \tau_\delta$, we have a predictable noise profile over the pulse window that can be compensated for by the algorithm. The optimized pulses have intervals where they change sign, resulting in the qubit's Bloch vector temporarily backtracking its Rabi oscillation trajectory (see Fig. 9). This *back-and-forth* pulse profile significantly improves the pulse's robustness, as evident from how small the J_{opt} value is compared to the initial pulse.

When $T \gg \tau_\delta$, we observe a trend where the nonzero part of the pulse is localized into a time window approaching that of a rectangular pulse at the maximum possible Rabi frequency shown by the green dot-dashed line in Fig. 2, which we refer to as “the narrow pulse.” We find this *squeezing* behavior expected as the most straightforward way to counteract the effect of the δ noise is to use a pulse with shorter duration (see Appendix D). The optimization fails to find a nontrivial optimized pulse shape since the short correlation time means that the δ noise does

not have a predictable profile over the pulse window for the algorithm to pulse-shape against.

As a comparison, the reported J_{opt} values for the narrow pulses are (0.096 ± 0.003) , (0.096 ± 0.003) , (0.098 ± 0.003) , (0.102 ± 0.004) , (0.119 ± 0.004) for $\tau_\delta = 100, 10, 1, 0.1, 0.01$, respectively. We observe that the optimized pulses in the large τ_δ cases achieve lower J_{opt} than the narrow pulses, showing that the QOC algorithm outperforms the trivial choice of narrow, high-frequency control pulses. On the other hand, the narrow pulses outperform the optimized pulses when τ_δ is small, which is to be expected since the algorithm tries to approach the narrow pulses for these cases, but fails due to the truncated basis.

B. Effects of the optimization options

In this subsection, we analyze the effect of the pulse-optimization options discussed in Sec. III C on the optimization results and optimized pulse robustness. Overall, these options affect the performance of the optimization algorithm and the resulting optimized pulse.

1. Pulse's degrees of freedom

We observe similar changes in the optimization outcomes, for the given τ_δ , N_c , and $\beta_{\max}$, as we relax the constraint on $\phi(t)$, as illustrated by Figs. 3(a)–3(c). When we allow $\phi(t)$ to take on any constant value, the optimization shifts $\phi(t)$ significantly away from the initial value of $\pi/2$, resulting in nonzero x components, as shown in Fig. 3(b). However, the value of J_{opt} does not significantly change, which is plausible considering that the δ noise has no preference in phase. When $\phi(t)$ is then allowed to vary in time, the pulse shape changes significantly, as shown by Fig. 3(c). However, the values of J_{opt} are generally higher than when $\phi(t)$ is fixed. By allowing $\phi(t)$ to be time dependent, we dramatically increase the complexity of the control space, making it harder for the algorithm to navigate despite the possibility of a better optimum. This is evident in Fig. 8, which shows that the transition to the subsequent superiteration is slowed down.

The result is similar for increasing the number of basis functions N_c per superiteration, as illustrated by Figs. 3(a) and 3(d). The value of J_{opt} may increase or decrease with no noticeable pattern from Fig. 7. Larger N_c means more variables to optimize, so the algorithm also suffers from the increased control space complexity. The results are evidently worse when we use both larger N_c and optimize $\phi(t)$ as a function of time, as shown by the last two rows of Fig. 7. This illustrates how reducing the control space complexity can be a useful strategy considering the computational constraint.

We may ask if it is preferable to relax the constraint on $\phi(t)$ or increase N_c . Our choice of $N_c = 10$ for fixed

$\phi(t)$ gives only one fewer variable to optimize per superiteration than allowing $\phi(t)$ to vary with time with $N_c = 5$ [see Eq. (11)], making them a good comparison point. Comparing cases (1.b.i.) versus (3.a.i.), and (1.b.ii.) versus (3.a.ii.) in Fig. 7, we see that the advantage of one over the other is inconsistent. As shown in Fig. 8, case (3.a.) optimizations generally iterate over fewer superiterations than case (1.b.) optimizations. This suggests that allowing $\phi(t)$ to vary with time is more desirable, as it takes fewer basis dressings and therefore a smaller total number of basis functions to produce a pulse with similar performance. The optimization may deal with the same number of variables, but relaxing the $\phi(t)$ constraint gives a larger freedom for the pulse shape, which enables lower J_{opt} values otherwise inaccessible by the algorithm.

2. Wiggles against wiggles

By increasing β_{max} , we allow the algorithm to add higher-frequency components into the pulse. As a result, we observe more wiggles in the optimized pulses, as can be seen by comparing Figs. 3(a) and 3(e). These extra wiggles are more pronounced in $\tau_\delta = 0.1, 0.01$ cases, despite being smaller than the large bumps resulting from the squeezing. In contrast, the regions outside the large bumps are nearly zero with a lower β_{max} . This suggests that the small wiggles are beneficial for the optimized pulse performance in the low τ_δ cases, as evident from the consistent J_{opt} decrease throughout the optimization runs and in agreement with the hypothesis we mentioned in Sec. III C. Therefore, increasing β_{max} provides a way to improve the optimization for low τ_δ cases without increasing the control space complexity.

No noticeable performance changes are observed for large τ_δ cases.

C. Experimental feasibility

To examine the experimental feasibility of the numerically optimized pulse, we sent selected pulses through a set of control devices commonly used in NV experiments [76]. A small variation in the generated pulse may significantly affect its performance, so it is necessary to ensure that the pulse generation is properly analyzed. We picked four optimized pulses with different features from the results shown in Fig. 6, then sent them to an arbitrary waveform generator (Tektronix AWG70002A with a DAC resolution of 10 bit, $V_{\text{pp}} = 500$ mV, and a time resolution of 1 ps), via our homebuilt control suite Qudi [118,119]. The pulses were amplitude modulated with a carrier frequency of 2.9 GHz, generated with a signal amplifier (Amplifier Model No. 60S1G4AM3 AR Germany with a frequency bandwidth of 0.7–4.2 GHz and a gain power of 60 W), and measured by an oscilloscope (Tektronix TDS6804B with a working bandwidth of 8 GHz).

The data is measured in volts over 1.2 μs with an active window of $T = 0.5$ μs . The experimentally generated pulses are obtained with a standard signal demodulation procedure. We multiply the pulses by the carrier waveform, then apply a low-pass filter to remove the resulting high-frequency oscillations, leaving only the experimental pulse waveform. Furthermore, a Savitzky-Golay filter is used to smooth out the resulting pulses. We then rescale the pulses to their numerical counterparts and horizontally shift the experimental pulses to align their active windows against the numerical pulses. Finally, we sampled the experimental pulse at the optimization sampling rate and calculated the corresponding cost-function value.

Figure 4 shows comparisons between the experimental and numerically optimized pulses alongside the ratio between the reported cost-function average of the experimentally generated pulse (J_{exp}) and the numerically optimized pulse (J_{num}). The pulse shapes match reasonably well, even in cases containing high-frequency components. Furthermore, the cost-function values of the experimental pulses are close to their numerical counterparts, showing that the small deviations do not significantly affect the experimental pulse performance. Our results show that the numerically optimized pulses can be reliably generated in a typical experimental setup, having considered the device's working capabilities during the optimization setup.

V. DISCUSSION AND OUTLOOK

In our optimization problem, which is typical for single NV centers in diamond, the δ noise dominates the spin dynamics, and the pulses are optimized to counteract it in particular. It is interesting to study the system dynamics as it suffers predominantly from the ϵ noise and analyze how the optimization performs in such a scenario. It is also possible to consider another way of optimizing the functions $f(t)$ and $\phi(t)$, for example, by expanding and optimizing $f_x = f(t) \cos[\phi(t)]$ and $f_y(t) = f(t) \sin[\phi(t)]$. This alternative may result in a better pulse performance as the optimized pulse features are inherently present in the pulse components.

As for the optimization parameters, using only two variations for a given parameter is insufficient to establish the dependency. A broader range of dependencies of the dCRAB optimization on the number of bases per superiteration and the maximum randomized basis parameters is expected to provide a better insight into the best parameter values to use. Increasing the function evaluation limit may also allow for optimizations with a larger number of variables to potentially reach a lower cost-function value. To obtain a faster convergence, utilizing other choices of bases may be beneficial [113].

Fine tuning the amplitude variation as one of the features of the optimization package QuOCS may also yield faster convergence. The choice of the initial guess pulse can also

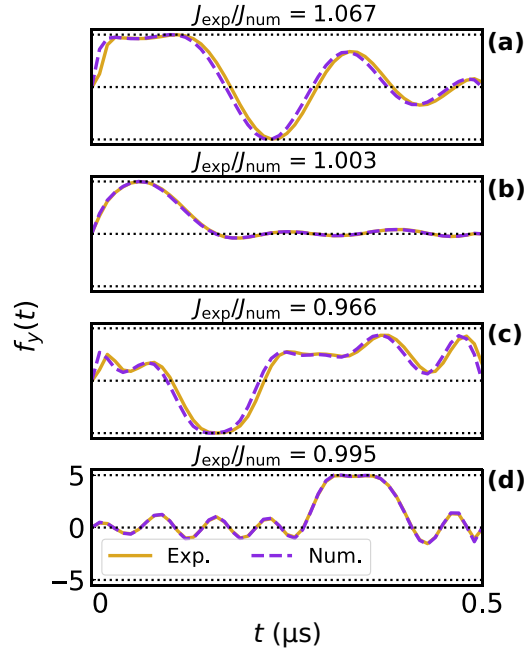


FIG. 4. Comparison of experimentally and numerically generated optimized pulse shapes $f_y(t)$ [$f_x(t) = 0$ for these cases] vs evolution time t for selected cases with $\phi = \pi/2$ and $N_c = 5$: (a) $\tau_\delta = 100, \beta_{\max} = 3$ (case 1.a.i.); (b) $\tau_\delta = 100, \beta_{\max} = 8$ (case 1.a.ii.); (c) $\tau_\delta = 0.01, \beta_{\max} = 3$ (case 1.a.i.); (d) $\tau_\delta = 0.01, \beta_{\max} = 8$ (case 1.a.ii.). The experimental data processing is discussed in the main text. On top of each plot is the ratio between the reported cost function average of the experimentally generated pulse (J_{exp}) and the numerically optimized pulse (J_{num}).

be critical. For instance, one may start with zero amplitude (no pulse) and let the algorithm build the optimized pulse ground up. As another example, we may do a *two-step optimization*, where the initial value is taken from the previous optimization with different parameters. The optimization outcome may also differ depending on the control objective. There are various possible expressions for J we may choose, depending on the goal. For example, one may use the gate fidelity when optimizing pulses for dynamical decoupling purposes.

Lastly, the fluctuating J should be considered if we aim for a value lower than the fluctuations, e.g., $J < 10^{-3}$, as the fluctuations are likely to prevent the algorithm from reaching convergence. This can be improved by increasing the sample size N_{sample} at the cost of a slower optimization.

VI. CONCLUSION

We have performed control optimization of qubit operations with environment-induced decoherence and control amplitude noise using the dCRAB method, demonstrating the experimental feasibility of such optimized operations. The optimizations improve the fidelity of spin-qubit

inversion, and the optimized control pulses outperform the standard nonoptimized rectangular control pulses. We have characterized how the optimized pulses behave with respect to the environmental noise characteristics and the noise correlation time, showing two different error-compensating mechanisms. Specifically, when the noise correlation time is much longer than the pulse duration, the optimized pulse has a complex shape that improves robustness, making use of the noise temporal correlations. On the contrary, when the noise correlation time is short, i.e., shorter than the pulse duration, the dominant error-compensating mechanism is pulse squeezing towards the shortest rectangular pulse at maximum amplitude. We have shown that the choice of optimization parameters and control constraints is key for the outcome of the optimization procedure and the experimental realization.

Our work serves as a guide and demonstrates what the expected forms and characteristics of the optimized pulses are, given realistic experimental constraints in a noisy spin environment. It can also be adapted for optimizing quantum sensing with an ensemble of NV centers, where pulse amplitude inhomogeneity is highly detrimental to performance.

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G.T.G., F.J., and R.S.S. conceptualized the work. H.M.L. and A.F. coded the numerical calculations. H.M.L. developed the simulation and optimization libraries and performed the numerical work. G.T.G. and H.M.L. worked on the theoretical analyses. R.S. and R.S.S. conceived the experiment. R.S. performed the measurements for the experimental pulses. F.J., G.T.G., H.M.L., R.S., and R.S.S. analyzed the data and drafted the manuscript. F.J. and M.A.M. acquired the project funding. F.J., G.T.G., M.A.M., and R.S.S. supervised the project. All authors read and contributed to the manuscript.

DATA AVAILABILITY

The datasets in this work are available from the corresponding author upon reasonable request. The processed data for the plots is publicly available [120].

APPENDIX A: RABI OSCILLATION AND DETUNING

The Rabi oscillation is ubiquitous in standard textbooks discussing two-level systems (e.g., see Refs. [121,122]).

Particularly, with Eq. (3), we have

$$\langle \sigma_z \rangle = \frac{\Omega_1^2 - \Delta^2}{\Omega_1^2 + \Delta^2} \sin^2 \left(\frac{\sqrt{\Omega_1^2 + \Delta^2}}{2} t \right) - \cos^2 \left(\frac{\sqrt{\Omega_1^2 + \Delta^2}}{2} t \right), \quad (\text{A1})$$

when the qubit starts in the $|0\rangle = (0 \ 1)^T$ state, corresponding to $\langle \sigma_z \rangle_{t=0} = -1$. It is evident that $\langle \sigma_z \rangle = 1$ is not possible for any t unless the detuning $\Delta = \omega - \omega_0$ is zero.

APPENDIX B: DETERMINATION OF THE OU PARAMETERS FOR THE δ NOISE

Firstly, we note that the derivations in this section have previously been done (see Ref. [57], which is our inspiration for our derivation here). We consider the qubit coherence ρ_{12} under the free evolution. Using Eq. (7) with $\Omega_1 = 0$, and von Neumann equation $\dot{\rho} = -i[\hat{H}, \rho]$, we obtain

$$\dot{\rho}_{12} = -i\delta\rho_{12},$$

whose solution is

$$\rho_{12}(t) = \rho_{12}(0) \exp \left[-i \int_0^t \delta(t') dt' \right].$$

Taking the average over experimental runs, and noting that $\rho_{12}(0)$ is the same for all runs, we have

$$\overline{\rho_{12}}(t) = \rho_{12}(0) \exp \left[-i \overline{\int_0^t \delta(t') dt'} \right].$$

For a Gaussian function $G(t)$, and an arbitrary function $f(t)$,

$$\overline{\exp \left[i \int_{t_0}^t f(t') G(t') dt' \right]} = \exp \left[-\frac{1}{2} \overline{\left(\int_{t_0}^t f(t') G(t') dt' \right)^2} \right].$$

We identify $t_0 = 0, f(t') = -1, G(t') = \delta(t')$ to get

$$\overline{\rho_{12}}(t) = \rho_{12}(0) e^{-\gamma(t)},$$

where

$$\begin{aligned} \gamma(t) &= \frac{1}{2} \overline{\left(\int_0^t (-1) \delta(t') dt' \right)^2} \\ &= \frac{1}{2} \int_0^t dt' \int_0^t dt'' \text{cov} \{ \delta(t'), \delta(t'') \}. \end{aligned}$$

The covariance $\text{cov} \{ X(t'), X(t'') \}$ of a fully relaxed OU process X is $\sigma^2 e^{-|t' - t''|/\tau}$, where $\sigma^2 = c\tau/2$. Furthermore,

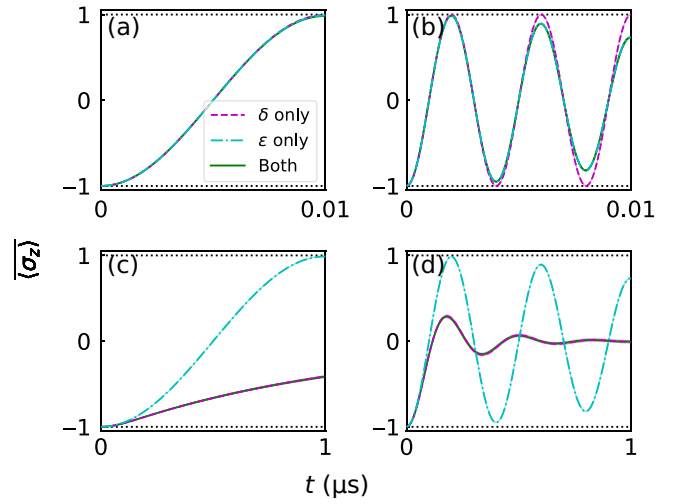


FIG. 5. Evolution of $\overline{\langle \sigma_z \rangle}$ in the presence of different noise sources— δ noise only, ϵ noise only, and both—for rectangular control pulses under different conditions: (a) short duration, small rotation phase; (b) short duration, large rotation phase; (c) long duration, small rotation phase; (d) long duration, long rotation phase. The value $\phi(t) = \pi/2$ is arbitrarily chosen and is the same for all simulations. The OU parameters of the δ noise, $\tau_\delta = 0.1 \mu\text{s}$ and $T_2^* = 0.1 \mu\text{s}$, are arbitrarily chosen such that the chosen pulse lengths and rotation phases exhibit different effects. Simulated with $N_{\text{sample}} = 1500, N_{\text{rep}} = 100$.

since $\text{cov}\{X, Y\} = \text{cov}\{Y, X\}$ we use the property that

$$\int_0^t dt' \int_0^t dt'' f(t', t'') = 2 \int_0^t dt' \int_0^{t'} dt'' f(t', t''),$$

given that $f(t', t'') = f(t'', t')$. Using these and working out the integral, we obtain

$$\gamma(t) = \sigma_\delta^2 \tau_\delta^2 \left(\frac{t}{\tau_\delta} + e^{-t/\tau_\delta} - 1 \right)$$

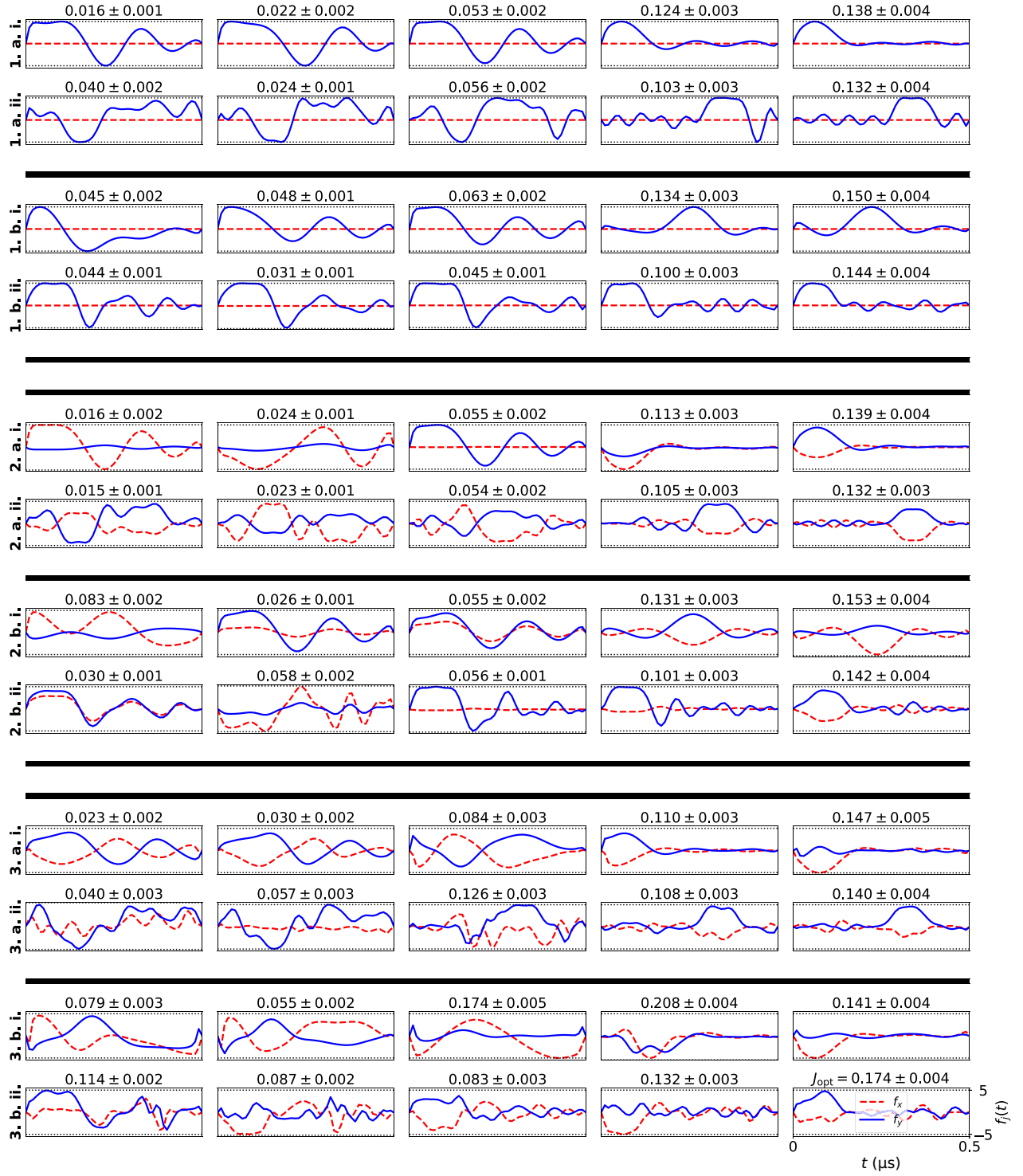
and thus

$$\overline{\rho_{12}}(t) = \rho_{12}(0) \exp \left[-\sigma_\delta^2 \tau_\delta^2 \left(\frac{t}{\tau_\delta} + e^{-t/\tau_\delta} - 1 \right) \right]. \quad (\text{B1})$$

For the evolution under a Hahn-echo sequence, we note that the coherence is conjugated each time a π pulse is applied, which rotates the Bloch vector by π over some axis in the x - y plane of the Bloch representation. Let T be the readout time, so the π pulse is applied at $T/2$. Let the pulse be *instantaneously* applied with some arbitrary phase shift $\phi = \alpha$ (in particular, $\phi = 0$ or $\phi = \pi/2$ is actually used for a Hahn-echo sequence). Then,

$$\rho_{21}^{(\text{after pulse})} = e^{i(\pi - 2\alpha)} \rho_{12}^{(\text{before pulse})}.$$

That is, the coherence ρ_{12} —evolving like how a “12” element evolves before the π pulse—“occupies” the “21” element after the π pulse and evolves like the “21” element,



1. a. i.	0.016 ± 0.001	0.022 ± 0.002	0.053 ± 0.002	0.124 ± 0.003	0.138 ± 0.004
1. a. ii.	0.040 ± 0.002	0.024 ± 0.001	0.056 ± 0.002	0.103 ± 0.003	0.132 ± 0.004
1. b. i.	0.045 ± 0.002	0.048 ± 0.001	0.063 ± 0.002	0.134 ± 0.003	0.150 ± 0.004
1. b. ii.	0.044 ± 0.001	0.031 ± 0.001	0.045 ± 0.001	0.100 ± 0.003	0.144 ± 0.004
2. a. i.	0.016 ± 0.002	0.024 ± 0.001	0.055 ± 0.002	0.113 ± 0.003	0.139 ± 0.004
2. a. ii.	0.015 ± 0.001	0.023 ± 0.001	0.054 ± 0.002	0.105 ± 0.003	0.132 ± 0.003
2. b. i.	0.083 ± 0.002	0.026 ± 0.001	0.055 ± 0.002	0.131 ± 0.003	0.153 ± 0.004
2. b. ii.	0.030 ± 0.001	0.058 ± 0.002	0.056 ± 0.001	0.101 ± 0.003	0.142 ± 0.004
3. a. i.	0.023 ± 0.002	0.030 ± 0.002	0.084 ± 0.003	0.110 ± 0.003	0.147 ± 0.005
3. a. ii.	0.040 ± 0.003	0.057 ± 0.003	0.126 ± 0.003	0.108 ± 0.003	0.140 ± 0.004
3. b. i.	0.079 ± 0.003	0.055 ± 0.002	0.174 ± 0.005	0.208 ± 0.004	0.141 ± 0.004
3. b. ii.	0.114 ± 0.002	0.087 ± 0.002	0.083 ± 0.003	0.132 ± 0.003	0.174 ± 0.004
	100	10	1	0.1	0.01
	τ_δ				

FIG. 7. Tile plot of the optimized cost function J_{opt} for different τ_δ and optimization options. The numbers being printed in white or black are solely for visibility. The optimization option codes are described in Fig. 6.

i.e., under the differential equation $\dot{\rho}_{21} = i\delta\rho_{21}$. Thus, the full equation of motion under the Hahn-echo sequence reads

$$\dot{\rho}_{12}^{\text{HE}} = \begin{cases} -i\delta\rho_{12}^{\text{HE}}, & 0 \leq t \leq T/2 \\ i\delta\rho_{12}^{\text{HE}}, & T/2 \leq t \leq T \end{cases},$$

where we have omitted $e^{i(\pi-2\alpha)}$ from both sides of the $T/2 < t < T$ case, showing that the choice of ϕ is irrelevant for the coherence. The solution to this differential equation at readout is

$$\rho_{12}^{\text{HE}}(T) = \rho_{12}(0) \exp \left[-i \int_0^{T/2} \delta(t') dt' + i \int_{T/2}^T \delta(t'') dt'' \right].$$

The rest of the derivation proceeds similarly to the free evolution case. We obtain

$$\begin{aligned} \overline{\rho_{12}^{\text{HE}}}(T) \\ = \rho_{12}(0) \exp \left[-\sigma_\delta^2 \tau_\delta^2 \left(\frac{T}{\tau_\delta} + 4e^{-T/2\tau_\delta} - e^{-T/\tau_\delta} - 3 \right) \right]. \end{aligned} \quad (\text{B2})$$

We then set the exponents in Eqs. (B1) and (B2) to be equal to one when the coherence lifetimes T_2^* and T_2^{HE} , respectively, are reached. Simultaneously solving these equations by substituting for σ_δ^2 yields Eq. (5), which can be solved to obtain τ_δ . The value of τ_δ can then be substituted to either of Eqs. (B1) and (B2) to obtain σ_δ^2 , and hence c_δ . Equation (6) uses the former.

The requirement that T_2^* and T_2^{HE} are obtained with short pulses, discussed in the main text, is a consequence of the assumption of ideal pulses in this derivation.

APPENDIX C: INTERPRETATION OF THE STOCHASTIC HAMILTONIAN

Usually, the observed dynamics of the system are represented by the state vector $|\psi\rangle$ or the density matrix ρ . The expectation value of an observable $\mathcal{O}$ is obtained by calculating $\langle\psi|\hat{\mathcal{O}}|\psi\rangle$ or $\text{tr}(\rho\hat{\mathcal{O}})$, which we can interpret as the average outcome when we repeat the measurements over an ensemble of identically prepared systems. However, with the presence of the OU noises, each sample of the system evolves differently depending on the exact form of the noises. For the j th evolution sample, the system evolves under the Hamiltonian $\hat{H}_j$ with the j th sample of the OU noises. We can expect to measure $\langle\mathcal{O}\rangle_j = \text{tr}(\rho_j\hat{\mathcal{O}}) = \langle\psi_j|\hat{\mathcal{O}}|\psi_j\rangle$, where $\rho_j = |\psi_j\rangle\langle\psi_j|$ is the density matrix evolving with $\hat{H}_j$ under the Schrödinger or the Liouville-von Neumann equation. Over the possible noise realizations, we expect to observe the average over these dynamics as given by the sample-averaged expected value $\overline{\langle\mathcal{O}\rangle} = \sum_{j=1}^{N_{\text{sample}}} \langle\mathcal{O}\rangle_j / N_{\text{sample}}$, where N_{sample} is the

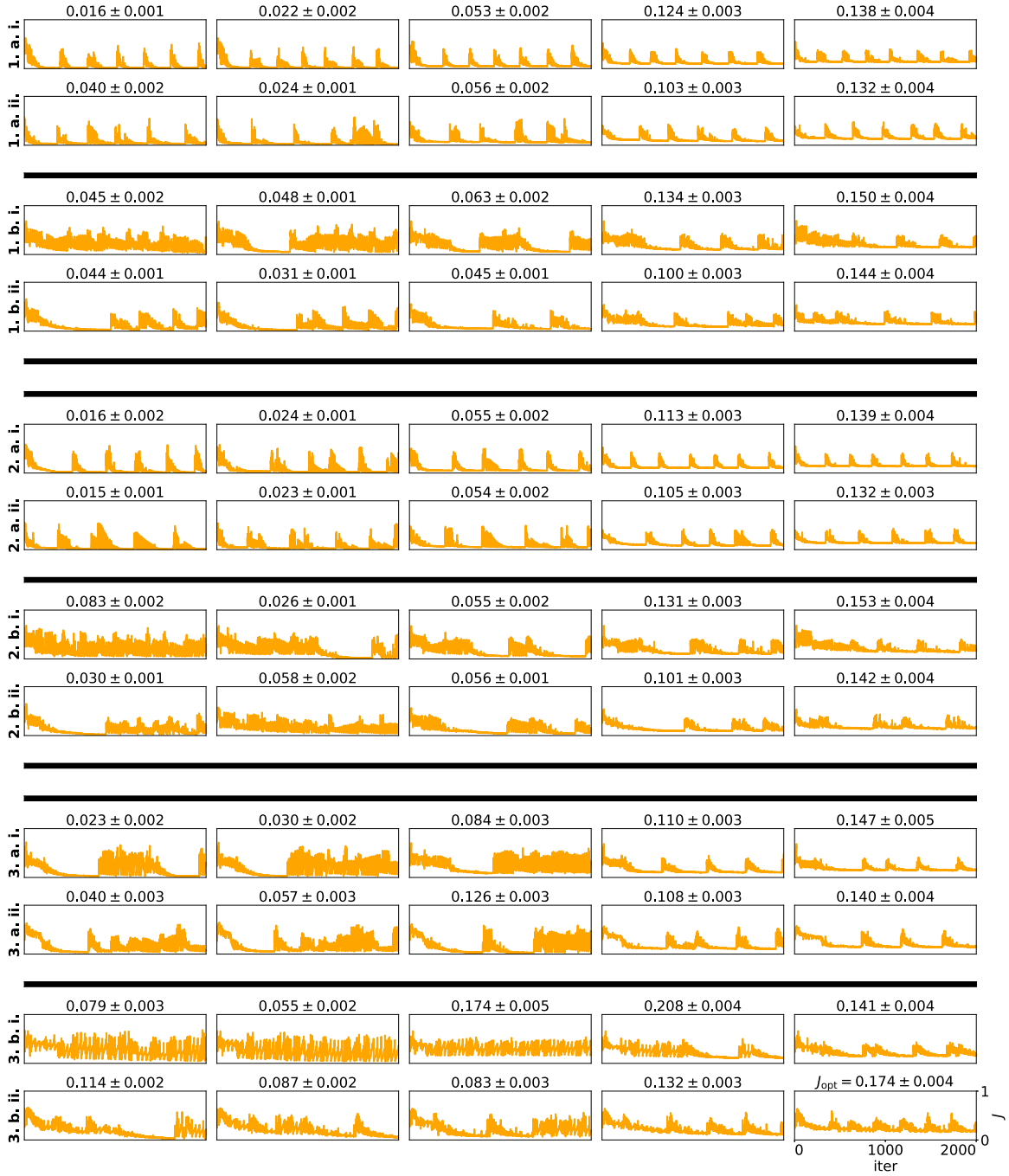


FIG. 8. Change in the cost function J over the optimization iterations. A sudden rise in J after converging to some value indicates a superiteration converging and the algorithm moving into the subsequent superiteration. Other features of the plots are the same as Fig. 6.

(large) number of samples. We note that

$$\begin{aligned} \overline{\langle \mathcal{O} \rangle} &= \frac{1}{N_{\text{sample}}} \sum_{j=1}^{N_{\text{sample}}} \langle \mathcal{O} \rangle_j = \text{tr} \left[\left(\frac{1}{N_{\text{sample}}} \sum_{j=1}^{N_{\text{sample}}} \rho_j \right) \hat{\mathcal{O}} \right] \\ &= \text{tr}(\bar{\rho} \hat{\mathcal{O}}), \end{aligned} \quad (\text{C1})$$

where we have defined the *sample-averaged density matrix* $\bar{\rho}$, which describes the dynamics expected over all the noise realizations.

Evidently, $\bar{\rho}$ and our discussion so far constitute the description of the dynamics of a mixed state [123,124], making $\bar{\rho}$ the mixed-state density matrix. We do not know which OU noise realization the qubit evolves under for the given evolution run. However, we do know that there

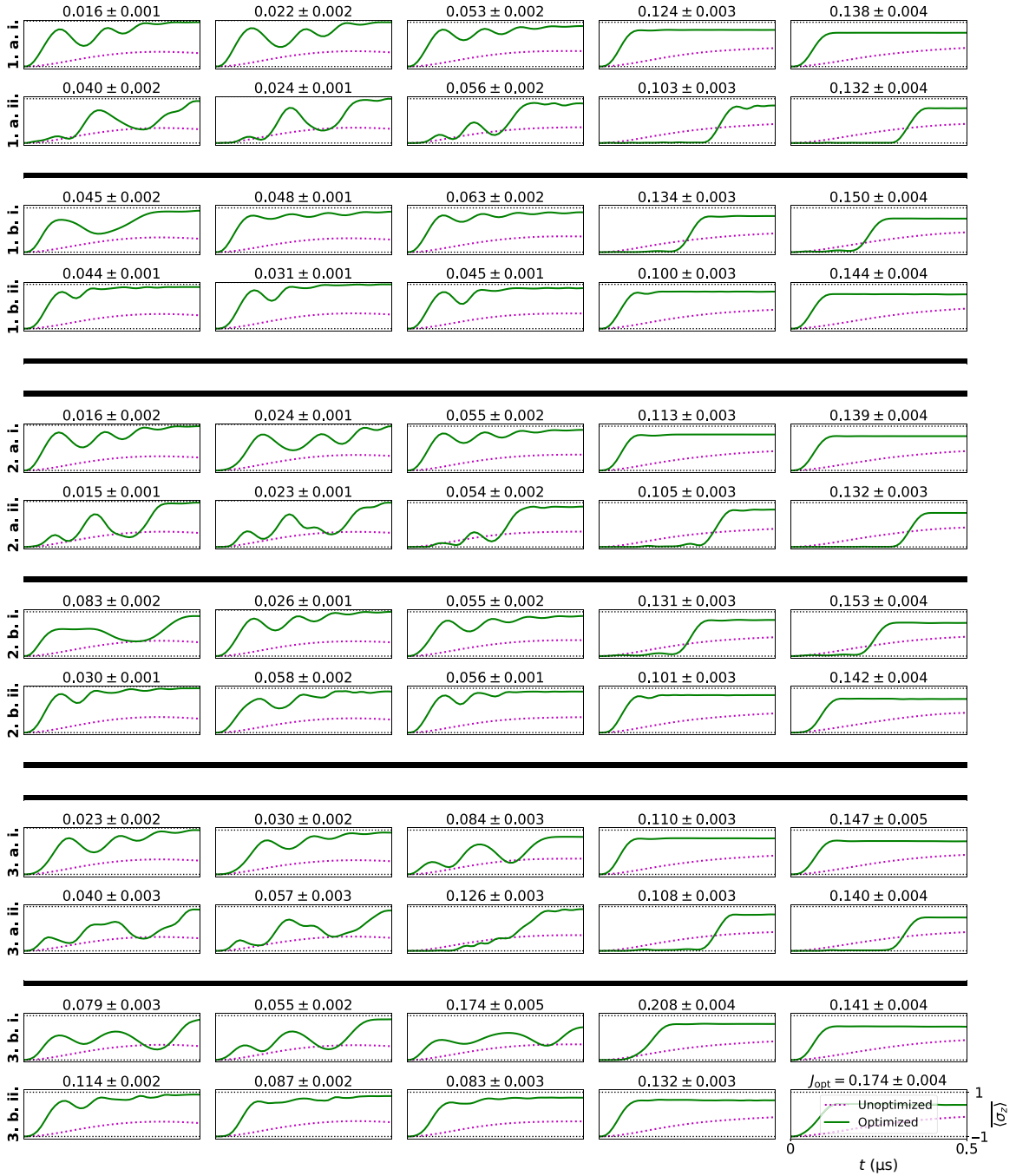


FIG. 9. Evolution of $\langle \sigma_z \rangle$ under the optimized pulses presented in Fig. 6, compared to the unoptimized version. The green solid lines represent the optimized evolution, while the magenta dotted lines represent the unoptimized evolution. The black dotted lines represent ± 1 . Other plot attributes are the same as Fig. 6.

is a $1/N_{\text{sample}}$ chance that the noises are one set among the possible realizations and that our qubit evolves into the corresponding final (pure) state. We may also view an instance of Hamiltonian the system evolves in as an element of a *Hamiltonian ensemble* [125]—the final state $\hat{\rho}$ is the average result of the system's evolution under the Hamiltonian ensemble.

APPENDIX D: THE δ NOISE VERSUS THE ϵ NOISE

As we illustrate in Fig. 1, the δ noise also affects the working of a control pulse, apart from causing decoherence. One question to address is whether the effect of the δ noise dominates over the ϵ noise for the given pulse.

We study how the δ and ϵ noise separately affect a control pulse. A control pulse is characterized by two of the following properties: the rotation phase, pulse duration, and pulse frequency, from which the third follows. Here we consider the evolution of $\langle\sigma_z\rangle$ under pulses of different duration and total rotation phases. The simulation is done with only one OU noise present, then with both present. The parameters of the δ noise and the initial phase ϕ of the control pulse are arbitrarily chosen. The values of the pulse properties are chosen to exhibit changes in behaviors of interest.

The simulation results are shown in Fig. 5. Figure 5(a) shows that when the pulse is short and does only a small rotation, the dynamics are not affected to any noticeable degree, and the qubit evolves very close to the ideal case where $\langle\sigma_z(t)\rangle = -\cos(\Omega_1 t)$ [see Eq. (A1)]. As the rotation phase is increased, as shown in Fig. 5(b), we see a deviation in the “ ϵ only” case and the “both” case, while the “ δ only” case stays close to the ideal case. This shows that the effect of the ϵ noise is dominant for large rotation phases. Moving on to Fig. 5(c), we see that when the rotation phase is small but the pulse duration is long, the δ noise is dominant. Finally, Fig. 5(d) shows the combined effect of both OU noises. In this case, we see a small deviation of the “both” case from the “ δ only” case, showing that the δ noise dominates over the dynamics in case (d). However, we cannot generally tell the dominance of one noise over the dynamics, as the dominance shown in Fig. 5(d) may be caused by the fact that the pulse duration is ten times that of τ_δ . This indeed makes an interesting problem in and of itself.

APPENDIX E: FULL VIEW OF THE OPTIMIZATION RESULTS

We compile all optimization results for the cases discussed in Sec. III. Figure 6 shows the x and y components of the dCRAB-optimized pulses. The comparison of the optimized cost function J_{opt} for different cases is compactly presented in Fig. 7. Meanwhile, Fig. 8 shows the change in the cost function over the optimization iterations. Lastly, Fig. 9 shows the optimized and unoptimized evolution of $\langle\sigma_z\rangle$ representing the population inversion.

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