

Synchronous manipulation of nuclear spins via boron-vacancy centers in hexagonal boron nitride

Fattah Sakuldee^{*} and Mehdi Abdi[†]

Wilczek Quantum Center, School of Physics and Astronomy, Shanghai Jiao Tong University, Shanghai 200240, China

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We develop a method for entangling operations on nuclear spins surrounding a negatively charged boron-vacancy (VB-center) point defect in hexagonal boron nitride (hBN). To this end, we propose to employ the electron spin of a VB center as a control qubit. We show that, in the presence of a background magnetic field and by applying control pulses, one can collectively manipulate the state of the nuclei with $\hat{U}_z$ and $\hat{U}_x$ rotations. These rotations can serve for implementing the synchronous three-qubit X , Z , and Hadamard gates. Through our numerical analyses considering realistic system parameters and decoherence effects, we demonstrate that these gates can be executed with high fidelities. Furthermore, as an example for the application of our toolbox, we use these collective gates to prepare the highly entangled Greenberger-Horne-Zeilinger states among the three nuclear spins with a fidelity of 0.99. By including electron decoherence effects, we find that the relative deviations of the gate fidelities from the noisy terms are negligibly small, demonstrating the noise resilience of our protocols. Our work can serve as the foundation for exploiting the nuclear spins in hBN in future quantum technological applications.

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I. INTRODUCTION

Nuclear spins are reliable solid-state candidates for storing quantum information because of their long coherence times [1–3]. Despite the difficulties in their accessibility for read-write and possibly other manipulations, several techniques have so far been proposed and even successfully implemented [4,5]. Devising versatile methods for not only transferring a quantum state to or from nuclear spins, but also for enabling various gate operations, can significantly push forward the idea of fault-tolerant quantum information processing in such platforms [6,7]. Such methods mostly rely on invoking a quantum mediator, namely, an electron spin interacting with the nuclei [8]. The color centers in solids are among the most reliable objects that can provide such access, thanks to the exhaustive control over the electron spin quantum mediator [9]. In particular, in diamond, several breakthroughs have been achieved, leading to profound developments in controlling nitrogen and carbon nuclear spins due to the high controllability of nitrogen vacancy (NV) centers [10–27]. For applications in

quantum computation, it has been recently shown that universal one- and two-qubit gates can be realized with NV centers [27,28], and the implementation of error correction in such gate operations has been devised [29]. Expansion of such fine controls to similar physical systems can significantly help to advance the field. Among other approaches, controlling nuclear spins in hexagonal structures of boron nitride via the embedded color centers seems a promising option [30].

The experimental observation of color centers in layered hexagonal boron nitride (hBN) structures [31–34] and the subsequent theoretical investigations [35,36] have identified highly controllable electron spins and brought about the quest to employ them for various quantum purposes. Negatively charged boron-vacancy centers (V_B^-), which in this paper we refer to as VB centers, are shown to be accessible for initialization and control via optical and microwave pulses [37]. The use of these centers in quantum applications has attracted great interest from the quantum community in the past few years. It is a promising physical platform for several purposes ranging from a host for quantum emitters [38–42] to quantum manipulation of other degrees of freedom and quantum sensing [43–52].

Even though the basics of a qubit in the manipulation (initialization, control, and readout) of the electron spin of a VB center in hBN have been established (see for example Refs. [32,37,53]), a reliable and scalable quantum information-processing strategy still requires further investigation and is an ongoing agenda. There remain

^{*}Contact author: fattah.sakuldee@sjtu.edu.cn

[†]Contact author: mehabdi@gmail.com

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several open possibilities to incorporate other degrees of freedom into the processing, which would lead to a more fruitful deployment of the potential of the mentioned system. Among other approaches, the nuclear spins in hBN offer a unique feature in systems hosting color centers; that is, all the stable isotopes of both nitrogen and boron have nonzero nuclear spins forming a lattice. This natural proximity of nuclei to the color center results in a large interaction with the electron spin, and yet in a regular fashion. Namely, given the lattice structure, the nuclear spins form an orderly spin structure, rather than being randomly located. These two features—strong coupling and the order—can be exploited to efficiently manipulate the quantum state of the nuclear spins. It is the purpose of this work to partially address this issue by putting forward a quantum toolbox composed of control gates for the collective manipulation of the three nearest nuclear spins surrounding a VB center in hBN.

The strong hyperfine interaction between the nuclear spins and the electron spin—dominant over other competing interactions [48,54]—combined with the ability to hyperpolarize the nuclear spins [55,56] and the excellent controllability of the electron spin in the VB center [32], presents a promising opportunity to achieve indirect control of nuclear spins via VB centers in hBN. The same principle can also be applied to the writing and reading processes of nuclear spin registers. Namely, since the central spin can be manipulated and read out efficiently [32,57], one can employ two-qubit gates to transfer the state between the nuclear spins and the electron spin, allowing the writing and reading processes of nuclear spins via the central electron spin as the mediator. In this work, we propose two crucial practical schemes from the perspective of the language of quantum computation, namely a synchronous nuclear spin qubit gates implementation and a preparation of three-qubit entangled state—the Greenberger-Horne-Zeilinger (GHZ) states.

We first demonstrate that the three ^{14}N nitrogen nuclear spins (in an isotopically purified sample), with the strongest coupling strength to the central spin, can be considered as three copies of an identical spin, and this can be further reduced to three identical copies of a qubit. By employing the symmetric nature of the hyperfine interaction and dynamical control techniques, we conceive entangling gates in which the reduced action on each nuclear spin is a rotation with the same phase across all the spins. In other words, three such identical qubits can be manipulated synchronously while assuming identical states. Such rotations are then exploited to conceive the Pauli gates X and Z , as well as the Hadamard gate. These provide the basic tools for quantum information processing from a quantum computation perspective. In addition to the synchronous control, we also consider the application of these entangling gates for the preparation of GHZ states, which are highly entangled states with various applications, e.g.,

in quantum sensing. Such states can be attained by the concatenation of spin initialization, the entangling gates, and a central spin measurement. The protocol leads to reduced operators on the nuclear spin subspace, mapping the initial nuclear state to two GHZ states with different phases, where one of them can be transformed into the other via appropriate postprocessing. The implication of the GHZ states opens another way to use the nuclear spins in hBN for quantum sensing.

The remainder of this paper is organized as follows. In Sec. II, we discuss the model of three nuclear spins coupled to a central electron spin and the mechanism for the realization of entangling gates used in our protocols. We use a two-level subspace of the electron spin as a control qubit subspace to manipulate the nuclear spins of the three adjacent nitrogen atoms. Later, we introduce an effective qubit subspace for the spin-1 system in Sec. III, where we demonstrate that the entangling gates can be considered as Pauli gates on such an effective subspace of each nuclear spin. The gate fidelities for realistic parameters of the system are numerically studied in Sec. IV. In Sec. V, we use the entangling gates for the preparation of GHZ states, achieving high fidelity. We then consider the effect of electron dephasing in Sec. VI, and finally, conclusions are given in Sec. VII.

II. FORMULATION

In this section, we discuss the relevant model of an electron spin and three ^{14}N nuclear spins clustered around a boron-vacancy center in hexagonal boron nitride. We show that by focusing on a two-level subspace of the central spin, one can construct collective entangling gates in which the effective phase on all nuclear spins is approximately uniform. Such collective gates are enabled by neglecting the fast-rotating terms and introducing a control term to the Hamiltonian, resulting in uniform coupling coefficients across all nuclear spins after the manipulation.

A. Boron vacancy in hexagonal boron nitride

The nuclear spins of the three nearest neighbors of a negatively charged boron-vacancy color center in hBN (VB center) strongly couples with the electron spin via Fermi contact (and small contribution of dipolar) interaction [32,54]. The coupling is anisotropic and thus allows one to systematically manipulate the nuclear spins when an appropriate external magnetic field is applied. The Hamiltonian describing the whole system is $\hat{H}_{\text{sys}} = \hat{H}_e + \hat{H}_n + \hat{H}_i$ with the following components ($\hbar = 1$):

$$\hat{H}_e = D_{\text{gs}}\hat{S}_z^2 + \gamma_e \mathbf{B} \cdot \mathbf{S}, \quad (1)$$

where D_{gs} is the zero-field splitting of the VB-center ground-state triplet and γ_e is the electron gyromagnetic ratio. Here, $\mathbf{B}$ is the vector of the background

magnetic field, while $\mathbf{S} = (\hat{S}_x, \hat{S}_y, \hat{S}_z)^T$ is the vector of spin-1 operators. The nuclear spins are also affected by the background magnetic field and the electric quadrupole interaction. Furthermore, they couple to each other through magnetic dipole-dipole and electric quadrupole interactions, which are negligibly small compared to the other frequencies. Hence, the Hamiltonian describing the dynamics of the nuclear spins reads

$$\hat{H}_n = - \sum_k \gamma_k \mathbf{B} \cdot \mathbf{I}_k, \quad (2)$$

where γ_k and $\mathbf{I}_k$ are the nuclear gyromagnetic ratio and the spin operator vector, respectively. The electron spin of the VB center couples to the nuclei via two different mechanisms. For the nearest-neighbor nuclear spins (three nitrogen atoms), the interaction is dominated by the Fermi contact, which is independent of the magnetic field orientation. This contribution is determined by the overlap of the wave function of the electron spin and the nuclear spins; namely, the coupling between the electron spin and the nuclear spin k is proportional to $|\Psi(\mathbf{r}_k)|^2 \mathbf{S} \cdot \mathbf{I}_k$, where $\Psi(\mathbf{r}_k)$ is the electron wave function at the location of the k th nuclear spin [56,58]. Given the localized nature of the defect orbitals (see for example Ref. [35]), only contributions from the three nearest nuclear spins are relevant, whereas the interactions with the other sites are negligibly small; see Fig. 1(a) for an illustration. The electron also couples to them, as well as to the farther spins, via dipole-dipole interactions, but the coupling strength is at least an order of magnitude smaller [54]. Therefore, we consider the four-spin system composed of the VB center and the three nearest-neighbor nitrogen nuclei as a computational unit. The interaction Hamiltonian reads

$$\hat{H}_i = \sum_k \mathbf{S} \cdot \mathbb{A}_k \cdot \mathbf{I}_k, \quad (3)$$

where $\mathbb{A}_k$ is the hyperfine tensor of the k th spin. Here, we have limited the interaction to the hyperfine interaction between the V_B^- center and the three nearest-neighbor nuclei and have omitted the other interactions. This is justified because of the much smaller coupling rates for the other interactions, as mentioned above. Both experimental data and computational studies suggest an anisotropy in the coupling of the VB center to the surrounding nuclei [54,59]. We will shortly show how this property can be exploited for the manipulation of the nuclear spins through the electron.

In fact, the hyperfine interaction matrix $\mathbb{A}_k$ inherits the geometric D_{3h} symmetry of the point defect and assumes

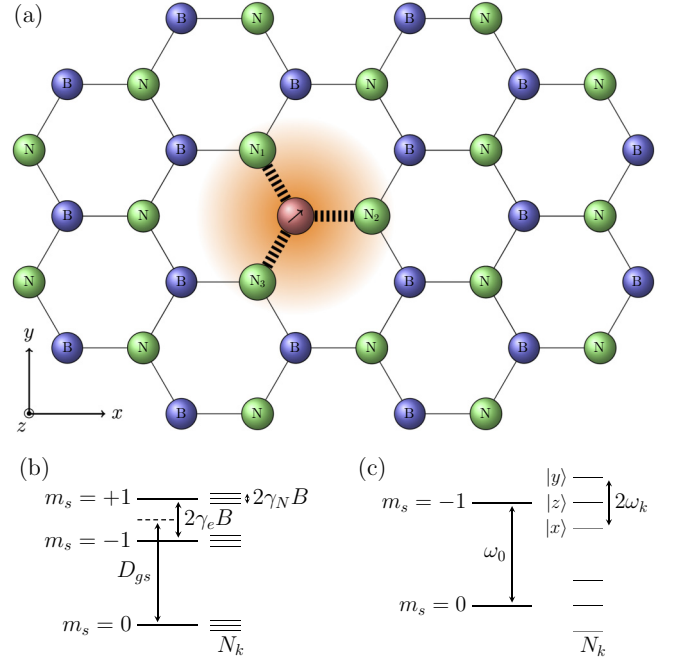


FIG. 1. The geometry of the VB center in hBN. (a) The electron spin of the boron vacancy (red ball) strongly couples to the three nearest nitrogen nuclear spins (green balls N_1 to N_3). These strong interactions are enabled by the Fermi contact (illustrated by the orange area around the VB center). Interactions between the electron spin and other sites are primarily dipolar and significantly weaker. A magnetic field is applied perpendicular to the lattice plane, i.e., along the z direction. (b) Energy level structure of the electron and any of the nuclei, which is symmetric under permutation of $\{N_k\}$ for $k = 1, 2, 3$. (c) The effective energy level structure in the reduced Hilbert space is shown, where the Larmor frequencies of spins N_k are shifted to $\omega_k = \gamma_N B + A_k^{zz}/2$ for a magnetic field along the z direction.

the following form [54]:

$$\mathbb{A}_k = \begin{pmatrix} A_k^{xx} & A_k^{xy} & 0 \\ A_k^{xy} & A_k^{yy} & 0 \\ 0 & 0 & A_k^{zz} \end{pmatrix}. \quad (4)$$

This can be represented as $\mathbb{A}_k = \mathbb{A}_k^\perp \oplus [A_k^{zz}]$. Therefore, the hyperfine interaction can be seen as a composition of a parallel $\hat{S}_z \sum_k A_k^{zz} \hat{I}_k^z$ and an in-plane $\sum_k \mathbf{S}_\perp \cdot \mathbb{A}_k^\perp \cdot \mathbf{I}_k^\perp$ interactions. Here, we have introduced the in-plane spin operators as $\mathbf{S}_\perp = (\hat{S}_x, \hat{S}_y)^T$ and $\mathbf{I}_k^\perp = (\hat{I}_k^x, \hat{I}_k^y)^T$. If the magnetic field vector is chosen such that the free-evolution part of the Hamiltonian, i.e., $\hat{H}_e + \hat{H}_n$, contains only in-plane or parallel spin components, the dynamics governed by the total Hamiltonian $\hat{H}_{\text{sys}}$ can then be considered as two separate independent branches of the evolution of parallel and in-plane components. Hence, the possibility of controlling these components independently is provided. This could be the case, for example, when one applies the magnetic field

in the parallel direction or the direction lying in the lattice plane.

In this work, we consider the magnetic field $\mathbf{B}$ pointing in the direction of the VB center's axis of symmetry, i.e., $\mathbf{B} = B\hat{z}$. We also assume that one can probe and manipulate the V_B^- electron subspace spanned by $\{|0\rangle, |-1\rangle\}$, the set of two lowest eigenstates of $\hat{S}_z$, which can be achieved by employing appropriate microwave drive frequencies (see for example Refs. [32,55]). By introducing the Pauli matrix $\hat{\sigma}_z = |0\rangle\langle 0| - |-1\rangle\langle -1|$ and similarly for $\hat{\sigma}_x$ and $\hat{\sigma}_y$, the relevant Hamiltonian, up to a global phase, in the two-level subspace reads

$$\hat{H} = -\frac{\omega_0}{2}\hat{\sigma}_z - \sum_k \left(\omega_k - \frac{A_k^{zz}}{2}\hat{\sigma}_z \right) \hat{I}_k^z + \frac{1}{\sqrt{2}} \sum_k \boldsymbol{\sigma}_\perp \cdot \mathbb{A}_k^\perp \cdot \mathbf{I}_k^\perp, \quad (5)$$

where $\omega_0 = D_{\text{gs}} - \gamma_e B$ and $\omega_k = \gamma_n B + A_k^{zz}/2$ are the effective Larmor frequencies of the electron and the k th nuclear spin, respectively [Figs. 1(b) and 1(c)]. Here, $\boldsymbol{\sigma}_\perp = (\hat{\sigma}_x, \hat{\sigma}_y)^T$ is a vector of the effective spin operators for the in-plane components.

B. Dynamical control

We now introduce control drives to the system that rotate the electron spin in the aforementioned subspace. The drive Hamiltonian thus reads $\hat{H}_C(t) = h_x(t)\hat{\sigma}_x + h_y(t)\hat{\sigma}_y$, with the functions $h_x(t)$ and $h_y(t)$ that need to be appropriately chosen. The total controlled Hamiltonian can then be described as

$$\hat{H}_{\text{tot}}(t) = \hat{H} + \hat{H}_C(t). \quad (6)$$

In our study, we assume that only one of the controls in a rotating frame with respect to $\hat{H}_e$ is applied at a time, and that both functions h_x and h_y are square pulses in that frame. These two assumptions simplify the problem and guarantee the filtered Hamiltonian form in the subsequent parts of this article (see Appendices A and B for details).

With these, one can rewrite the Hamiltonian of Eq. (6) in the rotating frame with respect to the free Hamiltonian $\hat{H}_0 = -\frac{\omega_0}{2}\hat{\sigma}_z - \sum_k \omega_k \hat{I}_k^z + \hat{H}_C(t)$ in the following form:

$$\tilde{H}(t) \approx \hat{H}_{\text{eff}}(t) + \hat{H}_{\text{RW,odd}}(t) + \hat{H}_{\text{CRW}}(t). \quad (7)$$

Here, the effective Hamiltonian is the approximation for $\tilde{H}(t)$ and is given as follows:

$$\begin{aligned} \hat{H}_{\text{eff}}(t) = & a_z F_z(t) \hat{\sigma}_z \sum_k \hat{I}_k^z + a_\perp F_x(t) \cos \Delta t \hat{\sigma}_x \sum_k \hat{I}_k^x \\ & + a_\perp F_y(t) \cos \Delta t \hat{\sigma}_y \sum_k \hat{I}_k^y. \end{aligned} \quad (8)$$

This is found by replacing the individual coupling coefficients in the first three terms with their averages:

$$\begin{aligned} \Delta = & \sum_k (\omega_0 - \omega_k) / 3, \\ a_z = & \frac{1}{6} \sum_k A_k^{zz}, \quad a_\perp = \frac{1}{6\sqrt{2}} \sum_k (A_k^{xx} + A_k^{yy}). \end{aligned}$$

In Eq. (8), the functions $F_\alpha(t)$ with $\alpha = x, y, z$ are filter functions induced by the control Hamiltonian $\hat{H}_C(t)$. Meanwhile, the rotating term with odd modulations is

$$\hat{H}_{\text{RW,odd}}(t) = \sum_k A_k^\perp \sin \Delta_k t \left(F_y(t) \hat{\sigma}_y \hat{I}_x - F_x(t) \hat{\sigma}_x \hat{I}_y \right), \quad (9)$$

and $\hat{H}_{\text{CRW}}(t)$ includes all counter-rotating terms. Both these latter contributions in the dynamics become vanishing with an appropriate choice of the filter functions (see below). Note that the homogeneity assumed here in introducing Δ , a_z , and $a_\perp$ results from the symmetric nature of the hyperfine interaction [54,55]. The derivation for the rotated Hamiltonian Eq. (7) and its full expression is given in Appendix A, while the filter function formulation can be found in Appendix B.

To obtain collective gates with desired rotations on the nuclear spins, one could choose the filter functions such that only one of the interactions in $\hat{H}_{\text{eff}}$ survives and the other two interactions, as well as the extra terms $\hat{H}_{\text{RW,odd}}(t) + \hat{H}_{\text{CRW}}(t)$, vanish. For instance, to single out the term $\hat{\sigma}_x \sum_k \hat{I}_k^x$, one should select the filter functions such that $F_z(t)$, $F_y(t)$, and $\hat{H}_{\text{RW,odd}}(t) + \hat{H}_{\text{CRW}}(t)$ average out to zero, as will be exemplified in the following.

In this paper, we discuss the construction of the following gates without loss of generality:

$$\hat{U}_z(\varphi) = \exp \left\{ -i\varphi \hat{\sigma}_z \sum_k \hat{I}_k^z \right\}, \quad (10a)$$

$$\hat{U}_x(\varphi) = \exp \left\{ -i\varphi \hat{\sigma}_x \sum_k \hat{I}_k^x \right\}. \quad (10b)$$

Rotations about the z axis require no control pulses and can be approximately obtained by choosing the magnetic field to be strong. In other words, when $|\Delta| \gg |A_k^{\alpha\beta}|/\sqrt{2}$ for $\alpha, \beta = x, y$, all interactions except for the $\hat{\sigma}_z \hat{I}_k^z$ terms in Eq. (7) become counter-rotating and thus negligible. In this case, arbitrary rotation angles are attainable by setting the evolution time to $t = \varphi/a_z$ such that

$$\exp \left\{ -i \int_0^t \tilde{H}(t) dt \right\} \approx \exp \left\{ -ia_z t \hat{\sigma}_z \sum_k \hat{I}_k^z \right\} = \hat{U}_z(\varphi).$$

In particular, the oscillation terms in $\hat{H}_{\text{eff}}(t)$ and $\hat{H}_{\text{RW,odd}}(t)$ with frequency Δ can be considered fast-rotating terms, which average out in the dynamics. Since $\hat{H}_{\text{CRW}}(t)$ contains oscillatory terms with frequency $\Sigma = \sum_k (\omega_0 + \omega_k)/3$, which is larger than Δ , the contribution from $\hat{H}_{\text{CRW}}(t)$ can also be neglected; see Appendix A.

The construction of $\hat{U}_x$ is more complicated, and it demands an active control ($\hat{H}_C(t) \neq 0$). In this work, we will employ a conventional Carr-Purcell-Meiboom-Gill (CPMG) sequence, as discussed below.

C. Preparation of $\hat{U}_x$

The CPMG sequence is implemented by inserting π rotations about $\hat{\sigma}_y$. For a sequence with period $T = 2\pi/\Omega$, such pulses are applied at times $T/4$ and $3T/4$, resulting in a set of filter functions:

$$F_x(t) = \sum_{k=0}^{\infty} \frac{4 \sin(k\pi/2)}{k\pi} \cos(k\Omega t), \quad (11)$$

where $F_y(t) = 1$ and $F_z(t) = F_x(t)$. Here, the pulse sequence is expressed in the rotating frame with respect to $\hat{H}_e$. We now choose the period such that the electron Larmor frequency is an odd multiple of the fundamental frequency $\Delta = p\Omega$. Suppose that the sequence completes at the N th period. One then has

$$\exp\left(-i \int_0^{NT} \tilde{H}(t) dt\right) \exp\left\{-i \left(\frac{4 \sin(p\pi/2) a_{\perp} N}{\Delta}\right) \hat{\sigma}_x \sum_k \hat{I}_k^x + C(NT)\right\}, \quad (12)$$

where $C(NT) = -i \int_0^{NT} \hat{H}_{\text{CRW}}(t) dt$ is the residue of counter-rotating terms. The terms with the filter functions $F_z(t)$ and $F_y(t)$ are averaged out to zero, while the integral of $\hat{H}_{\text{RW,odd}}(t)$ vanishes due to the orthogonality of trigonometric functions.

The contribution $C(NT)$ is relatively small compared to the main contribution since the effective coupling coefficients are small compared to $a_{\perp}$ and the average of the oscillation terms with counter-rotating frequencies $\Sigma_k = \omega_0 + \omega_k$ are off-resonant. We avoid long-term behavior when such an effect can accumulate and alter the observed results. The exact form of the remaining term $C(NT)$ is complicated, but it can be made small by choosing appropriate values of p and other parameters, e.g., B and N . In other words, with appropriate choices of parameters, one can safely remove the contribution $C(NT)$ in some relevant situations, which will be exemplified by the numerical calculations in Sec. V C.

With this scheme, the target rotation $\hat{U}_x(\varphi)$ is attained with a finite resolution. Namely, for a given rotation angle

φ in the preparation with N periods of CPMG pulses, one has $|\varphi| = N\delta_{\Delta}$, with $\delta_{\Delta} = 4a_{\perp}/|\Delta|$. This suggests that Δ exhibits a resolution parameter and N becomes the counting factor for a given phase φ . To achieve a reasonable resolution, one can choose the magnetic field to be large; however, having a large Δ may cause another practical issue; namely, the frequency of the control pulses $\Omega = \Delta/p$ will need to become large. This largely depends on the limitations of the experimental setups, meaning that the ability to vary φ is also limited by the ability to implement the control sequences.

III. SPIN ALGEBRA AND COLLECTIVE GATES

Before demonstrating the gate implementations, let us examine the algebraic structure of the nuclear spins. We begin by discussing local manipulations of a two-level subspace embedded in each nuclear spin manifold and show that such manipulations can be implemented collectively using our devised gates. Later, we demonstrate that one can realize a collective Pauli group on three nuclear two-level systems, and finally, we use the preparation of GHZ states in the nuclei to exemplify the potential of our framework.

A. Two-level subsystems

First, for clarity, let us define some notation as follows. On the electron spin, let $|\pm\rangle = (|0\rangle \pm |-1\rangle)/\sqrt{2}$. Let $|m_I\rangle_k$ denote an eigenstate of $\hat{I}_k^z$ associated with the eigenvalues $m_I = 0, \pm 1$ for spin k . Now, for the nuclear spins, we introduce $|z\rangle_k = |0\rangle_k$, $|x\rangle_k = (|1\rangle_k - |-1\rangle_k)/\sqrt{2}$, and $|y\rangle_k = (|1\rangle_k + |-1\rangle_k)/\sqrt{2}$. With this nomenclature, one observes that

$$\hat{I}_k^x = \hat{X}_k^{yz} := |y\rangle_k \langle z| + |z\rangle_k \langle y|, \quad (13a)$$

$$\hat{I}_k^y = -\hat{Y}_k^{zx} := i|z\rangle_k \langle x| - i|x\rangle_k \langle z|, \quad (13b)$$

$$\hat{I}_k^z = \hat{X}_k^{xy} := |x\rangle_k \langle y| + |y\rangle_k \langle x|. \quad (13c)$$

In other words, each spin operator acts as an X or Y gate on two orthogonal states apart from the state associated with the operator label; e.g., the operator $\hat{I}_k^x$ swaps between $|y\rangle_k$ and $|z\rangle_k$ but maps $|x\rangle_k$ to zero.

By employing Euler's formula for spin-1 operators, this observation leads to

$$\exp(-i\varphi \hat{I}_k^x) = \hat{P}_k^x + \cos \varphi \hat{P}_k^{yz} - i \sin \varphi \hat{X}_k^{yz}, \quad (14)$$

$$\exp(-i\varphi \hat{I}_k^y) = \hat{P}_k^y + \cos \varphi \hat{P}_k^{zx} + i \sin \varphi \hat{Y}_k^{zx}, \quad (15)$$

$$\exp(-i\varphi \hat{I}_k^z) = \hat{P}_k^z + \cos \varphi \hat{P}_k^{xy} - i \sin \varphi \hat{X}_k^{xy}, \quad (16)$$

where $\hat{P}_k^{\alpha} = |\alpha\rangle_k \langle \alpha|$ are the projective operators and $\hat{P}_k^{\alpha\beta} = \hat{P}_k^{\alpha} + \hat{P}_k^{\beta}$ for $\alpha, \beta = x, y, z$. From these expressions, one can interpret that an exponential operator generated by

I_k^α maintains the state $|\alpha\rangle_k$, whereas it shuffles the other two states, with the transition amplitudes depending on the phase φ , as seen in the coefficients of $\hat{P}_k^{\alpha\beta}$ and $\hat{X}_k^{\alpha\beta}$. Note that one can rewrite Eqs. (10a) and (10b) as

$$\hat{U}_z(\varphi) = |0\rangle\langle 0| \otimes \prod_{k=1}^3 e^{-i\varphi \hat{I}_k^z} + |-1\rangle\langle -1| \otimes \prod_{k=1}^3 e^{i\varphi \hat{I}_k^z}, \quad (17a)$$

$$\hat{U}_x(\varphi) = |+\rangle\langle +| \otimes \prod_{k=1}^3 e^{-i\varphi \hat{I}_k^x} + |-\rangle\langle -| \otimes \prod_{k=1}^3 e^{i\varphi \hat{I}_k^x}. \quad (17b)$$

In this sense, it is possible to employ the entangling gates $\hat{U}_z(\varphi)$ and $\hat{U}_x(\varphi)$ to manipulate only two of the three states on each spin, with the aid of the electron state $|0\rangle$ or $|+\rangle$ as an auxiliary qubit. The effect on the three spins is the same, thanks to the structure of the conditioned map on the nuclear spins. That is, for a given electron state $|0\rangle$ or $|+\rangle$, all nuclear spins will be rotated synchronously with the same phase φ .

With the above formulation, one can employ any pair of states in $\{|x\rangle_k, |y\rangle_k, |z\rangle_k\}$ as basis states for a qubit, allowing us to construct a three-qubit subspace from the system of three nuclear spins. Moreover, for any nuclear spin k , since $\hat{U}_\alpha(\varphi)$ for $\alpha = x, y, z$ concerns only one fixed axis α , one can manipulate each type of qubit subspace separately, synchronously on three nuclear spins at once, while leaving the components in the perpendicular subspace invariant. For instance, one can choose a Hilbert subspace spanned by $\{|y\rangle_k, |z\rangle_k\}_k$ (which throughout this paper we will call either the yz subspace or $\mathcal{H}_{yz}$ for short) on which either $\hat{U}_z(\varphi)$ or $\hat{U}_x(\varphi)$ can be employed to manipulate the state within the subspace. This can be done by setting the initial state in $\mathcal{H}_{yz}$, or for the case of an initial mixed state, the density matrix on such a Hilbert subspace $\mathcal{H}_{yz}$. A similar framework is also applicable for the other two, $\mathcal{H}_{zx}$ and $\mathcal{H}_{xy}$. In the following, and throughout this article, we use $\mathcal{H}_{yz}$ as an example and demonstrate how one can construct three-qubit synchronous gates.

B. Synchronous Pauli group

We now use the observations above for the preparation of qubit Z , X , and Hadamard gates on the subspace $\mathcal{H}_{yz}$. For instance, one can consider the nuclear spin subspace spanned by $\{|y\rangle_k, |z\rangle_k\}_k$ and treat it as a collective two-level Hilbert space. In our analyses, we adopt the compact notation $\hat{A}_{\alpha\beta} = \hat{A}_1^{\alpha\beta} \hat{A}_2^{\alpha\beta} \hat{A}_3^{\alpha\beta}$ for a collective of the operator $\hat{A}$. We call this type of operator, in which the action on each nuclear spin is identical, a synchronous gate. For the operator $\hat{X}_{yz}$, it can be easily obtained from the restriction of the $\hat{U}_x(\pi/2)$ on the mentioned subspace $\mathcal{H}_{yz}$. Specifically, we

have

$$\begin{aligned} \hat{U}_x(\pi/2) \left(\mathbb{1} \otimes \hat{P}_{yz} \right) &= |+\rangle\langle +| \otimes \prod_{k=1}^3 \left[\left(\hat{P}_k^x - i\hat{X}_k^{yz} \right) \hat{P}_k^{yz} \right] \\ &\quad + |-\rangle\langle -| \otimes \prod_{k=1}^3 \left[\left(\hat{P}_k^x + i\hat{X}_k^{yz} \right) \hat{P}_k^{yz} \right] \\ &= i \left(\hat{\sigma}_x \otimes \hat{X}_1^{yz} \hat{X}_2^{yz} \hat{X}_3^{yz} \right) = i\hat{\sigma}_x \otimes \hat{X}_{yz}. \end{aligned} \quad (18)$$

The projection on the right-hand side in the first expression is employed to represent the preparation of the initial nuclear spin state in the yz subspace. With another local gate $-i\hat{\sigma}_x$ on the electron part, the restriction of the action $(-i\hat{\sigma}_x \otimes \mathbb{1})\hat{U}_x(\pi/2)$ on the yz nuclear collective subspace, i.e.,

$$(-i\hat{\sigma}_x \otimes \mathbb{1})\hat{U}_x(\pi/2) \left(\mathbb{1} \otimes \hat{P}_{yz} \right) = \mathbb{1} \otimes \hat{X}_{yz},$$

can be considered as a collective X gate, as expected.

For the Z gate on the same subspace, from the relation

$$\begin{aligned} \hat{U}_z(\pi) \left(\mathbb{1} \otimes \hat{P}_{yz} \right) &= |0\rangle\langle 0| \otimes \prod_{k=1}^3 \left[\left(\hat{P}_k^z - \hat{P}_k^{xy} \right) \hat{P}_k^{yz} \right] \\ &\quad + |-1\rangle\langle -1| \otimes \prod_{k=1}^3 \left[\left(\hat{P}_k^z + \hat{P}_k^{xy} \right) \hat{P}_k^{yz} \right] \\ &= -\mathbb{1} \otimes \hat{Z}_{yz}, \end{aligned} \quad (19)$$

or the restriction of $-\hat{U}_z(\pi)$ on the yz nuclear collective subspace can be considered as a collective Z gate, as claimed. With these $\hat{X}_{yz}$ and $\hat{Z}_{yz}$, one automatically has a product Pauli group on three qubits, with the relation

$$\hat{Z}_{yz}\hat{X}_{yz} = -\hat{X}_{yz}\hat{Z}_{yz},$$

setting gate set for the collective three-qubit computation.

In addition to X and Z gates, by varying the phase φ , one can also use the same technique to prepare a Hadamard gate:

$$\hat{H}_{yz} = \hat{H}_1^{yz} \hat{H}_2^{yz} \hat{H}_3^{yz} = 2^{-3/2} \prod_{k=1}^3 \left(\hat{P}_{yz} + i\hat{X}_k^{yz} \right). \quad (20)$$

This can be prepared from Eq. (14), whose reduced action on yz collective subspace $(|- \rangle \langle -| \otimes \hat{P}_{yz}) \hat{U}_x(\pi/4)$ resembles the gate $\hat{H}_{yz}$. In particular, one can write

$$\begin{aligned} \hat{U}_x(\pi/4) (|- \rangle \langle -| \otimes \hat{P}_{yz}) \\ = |- \rangle \langle -| \otimes \prod_{k=1}^3 \left\{ \left[\hat{P}_k^x + \frac{\hat{P}_k^{yz} + i\hat{X}_k^{yz}}{\sqrt{2}} \right] \hat{P}_k^{yz} \right\} \\ = |- \rangle \langle -| \otimes \hat{H}_{yz}. \end{aligned} \quad (21)$$

Suppose that one can rotate the central spin initial state to $|- \rangle$, the action Eq. (20) on the nuclear spins simply follows Eq. (21) as claimed. A similar technique is also implementable for the preparation of a rotation gate

$$\hat{R}_{yz}(\varphi) = \prod_{k=1}^3 \left(\cos \varphi \hat{P}_{yz} + i \sin \varphi \hat{X}_{yz} \right), \quad (22)$$

for various phases φ . With Pauli groups generated by $\hat{X}_{yz}$ and $\hat{Z}_{yz}$ and the collection of rotation gates $\hat{R}_{yz}(\varphi)$ above, in principle, one is allowed to manipulate the three nuclear spin qubits synchronously in an arbitrary fashion. This technique will be promising for fault-tolerant information encoding.

In summary, through $\hat{U}_\alpha(\varphi)$ and the initialization of all nuclear spins to an identical state in a particular subspace $\mathcal{H}_{\alpha\beta}$, one can employ the three nuclear spins as three copies of identical qubits, where one can manipulate these three qubits synchronously. Since one can employ one subspace $\mathcal{H}_{\alpha\beta}$ at a time and any two subspaces overlap, e.g., $\mathcal{H}_{\alpha\beta} \cap \mathcal{H}_{\beta\gamma} \neq \emptyset$, one can use the whole Hilbert space of the system by a concatenation of the gates on different subspaces, e.g., $\hat{X}_{\alpha\beta} \hat{X}_{\beta\gamma}$. This allows us to simplify the manipulation of the three qubits into qubit manipulation problems. Another interesting topic is to extend the consideration from the construction of Pauli gates to other gates, which, combined with the Pauli gates and rotation gates we introduced, constitute a set of universal qubit gates. Further development in this direction is out of the scope of the current work and invites a dedicated investigation.

IV. GATE FIDELITIES

Next, we numerically calculate the fidelity of our constructed gates using the real parameters observed in experiments to signify that our protocols are promising in real-world applications. To determine the quality of the derived gates, we investigate the exact evolution governed by $\tilde{H}(t)$ given in Eq. (7). To gauge the quality of the gates, we consider a relative average gate fidelity defined by $F_R(\hat{E}, \hat{V}) = F(\hat{V}^\dagger \hat{E})/F(\hat{V}^\dagger \hat{V})$, where $F(\hat{E}) = \int d\psi |\langle \psi | \hat{E} | \psi \rangle|^2$ is the average gate fidelity of the channel $\mathcal{E} = \hat{E} \cdot \hat{E}^\dagger$ [60,61].

The integration is performed over the uniform (Haar) measure $d\psi$ on the full Hilbert space of electron and nuclear spins. Here, $\hat{E}$ and $\hat{V}$ are operators on such a Hilbert space, and $\hat{V}$ is a projected unitary operator on $\mathbb{1} \otimes \mathcal{H}_{yz} \equiv \mathcal{H}_{yz}$, namely $\hat{V} = (\mathbb{1} \otimes \hat{P}_{yz}) \hat{V} (\mathbb{1} \otimes \hat{P}_{yz})$. We use the relative average gate fidelity rather than the average gate fidelity since we are working on the collective qubit subspace where each nuclear spin is reduced to a two-level system, as formulated in Sec. III A. Note that the target operator $\hat{V}$ is not full rank but a unitary operator on the concerned subspace, and thus the renormalization of the average is necessary.

For the preparation of the X gate, in parallel to the relation Eq. (18), we set

$$\begin{aligned} \hat{E} &= \hat{U}_x(\pi/2) (\mathbb{1} \otimes \hat{P}_{yz}), \\ \hat{V} &= i\hat{\sigma}_x \otimes \hat{X}_{yz}. \end{aligned}$$

As mentioned in the previous section, the preparation of $\hat{U}_x$ involves various parameters, which one can choose to achieve a better quality of the gate. Throughout this article, the numerical results were performed using the QUTIP package [62,63] on PYTHON. In particular, we employ the built-in functions to compute average gate fidelities as well as the state fidelities in the following sections.

In Fig. 2(a), the maxima of relative average gate fidelity for the X gate are displayed for various N and p values, where the magnetic field strengths are set from the relation between the revolution step N and the target phase $\varphi = \pi/2$. Technically, from the relation $|\varphi| = 4Na_\perp/|\Delta|$, we choose the magnetic field above the crossing point ($\Delta > 0$):

$$B_{\text{op}}(\varphi, N) = \frac{1}{\gamma_e - \gamma_n} \left(\frac{4Na_\perp}{\varphi} + D_{\text{gs}} + a_z \right). \quad (23)$$

One can observe in Fig. 2(a) a region where the fidelity is very high, exceeding 0.98. We note that for finer resolution δ_Δ , one needs to operate at higher magnetic field strength. For example, for a larger number of revolutions $N = 100$, one can have $B_{\text{op}}(\pi/2, 100) = 567$ mT and $B_{\text{op}}(\pi/2, 200) = 1.01$ T. In Fig. 2(b), we demonstrate the evolution of the fidelity for various N values, where one can observe the maxima around $t = 4a_\perp N/\Delta$, which is 40.43 ns, predicted by the entangling gate $\hat{U}_x(\pi/2)$. At $N = 50$, $\Omega = \Delta/5$, and with $B = 345$ mT, one can obtain 0.9908 fidelity for the preparation of $\hat{X}_{yz}$. The deviations of the optimal times—the times at which the maxima occur—are relatively small and can be neglected for high enough N . For instance, we observe that the deviation for $N = 50$ is less than the resolution of the calculations. Therefore, we will use the parameters $p = 5$ and $N = 50$ for the examples of the $\hat{X}_{yz}$ preparation throughout the rest of the paper.

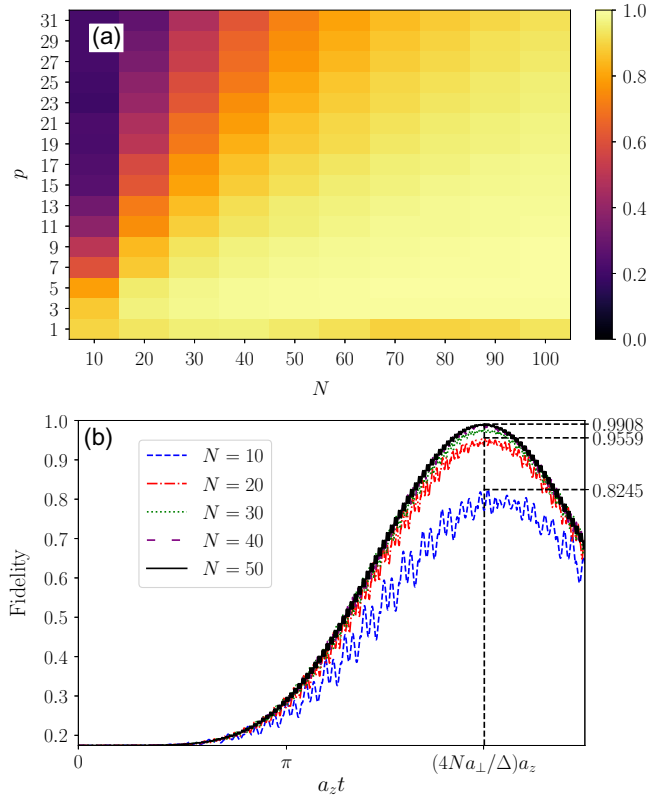


FIG. 2. Relative average gate fidelity for the X gate derived from the exact dynamics $\tilde{H}(t)$ in Eq. (7). (a) The maxima for various N and p values indicate the region where one can achieve fidelity close to unity (the light-shaded area). The colors in (a) represent fidelity values ranging from 0 (dark purple) to 1 (light yellow). (b) Time-evolution buildup of the X gate for the first few instances for the case $p = 5$. The corresponding magnetic field can be computed as a function of N by Eq. (23). One can achieve a fidelity as high as 0.9908 for $N = 50$ at the evolution time close to $t = 4Na_{\perp}/\Delta = 40.43$ ns (the vertical dashed line) predicted by the expected operator $\hat{U}_x(\pi/2)$. The horizontal dashed lines indicate the maxima for $N = 10, 20$, and 50 .

Similarly, for the preparation of the Z gate, in connection to Eq. (19) we set

$$\begin{aligned}\hat{E} &= \hat{U}_z(\pi) (\mathbb{1} \otimes \hat{P}_{yz}), \\ \hat{V} &= -\mathbb{1} \otimes \hat{Z}_{yz}.\end{aligned}$$

In Fig. 3, the relative average gate fidelity for the Z gate given by this protocol is shown for various magnetic fields. One can observe that at zero field, the relative average gate fidelity is small due to the contribution becoming non-negligible from the rotating and counter-rotating terms. Even for the zero-field case, where the value of the Larmor frequency $|\Delta| \sim 3447 \cdot 2\pi \times \text{MHz}$ is much larger than the hyperfine coupling rates $|A_k^{\alpha\beta}| \sim 20\text{--}80 \cdot 2\pi \times \text{MHz}$ for $\alpha, \beta = x, y$, the accumulation of

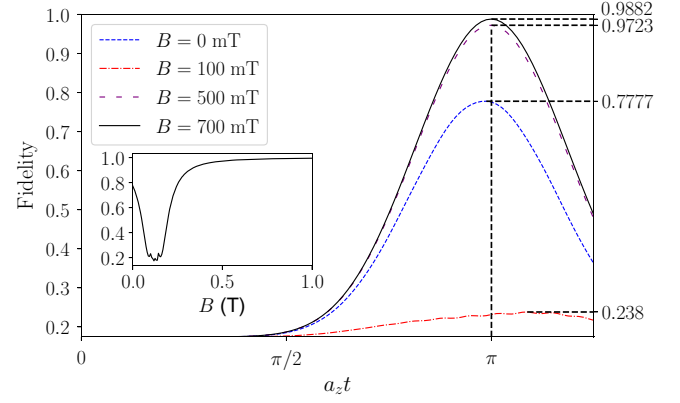


FIG. 3. Relative average gate fidelity for the Z gate derived from the exact dynamics $\tilde{H}(t)$ for various magnetic fields. The inset shows the fidelity at the end of the evolution $t = \pi a_z^{-1} = 20.76$ ns for magnetic field strengths between 0 and 1 T. The horizontal dashed lines indicate the maxima, while the vertical dashed line represents the target optimal time $t = \pi a_z^{-1}$ predicted by $U_z(\pi)$. Here, no deviation from the target optimal time for large magnetic fields ($B = 500$ and 700 mT) is observable.

errors from the counter-rotating terms and the odd rotating terms in Eq. (7) in the dynamics of in-plane interaction is still visible and results in a rather low relative average gate fidelity. At $B = 100$ mT, Δ becomes comparable to the in-plane interaction, and the observed fidelity is drastically reduced. Nevertheless, as predicted by our theory, the fidelity increases when the magnetic field is larger (see the inset in Fig. 3) and can reach about 0.9723 for $B = 500$ mT and 0.9882 for $B = 700$ mT. In addition, we also observe no deviation in optimal times from the target value $t = \pi a_z^{-1} = 20.76$ ns for high magnetic fields $B = 500$ and 700 mT. Finally, for the Hadamard gate Eq. (21), we set

$$\begin{aligned}\hat{E} &= \hat{U}_x(\pi/4) (|-\rangle\langle -| \otimes \hat{P}_{yz}), \\ \hat{V} &= |-\rangle\langle -| \otimes \hat{H}_{yz}.\end{aligned}$$

We note that in this case, in addition to the yz subspace for nuclear spins, the initial state is also concentrated in the electron spin subspace with respect to the state $|-\rangle$. The maximum relative average gate fidelity for this gate given by this protocol is shown in Fig. 4(a) for various harmonic orders p and numbers of revolutions N , and hence the operational magnetic field. In Fig. 4(b), the fidelity is shown as a function of time for the parameters of $\hat{U}_x$ set as $p = 5$ and various N , where the maxima can be found around $t = 4a_{\perp}N/\Delta = 20.21$ ns.

First, in Fig. 4(a), we observe an oscillation in p of the maximum fidelity, with clear visibility for high p . This arises from the factor $\sin(p\pi/2)$ in Eq. (12), which alters the sign of the phase φ depending on p ,

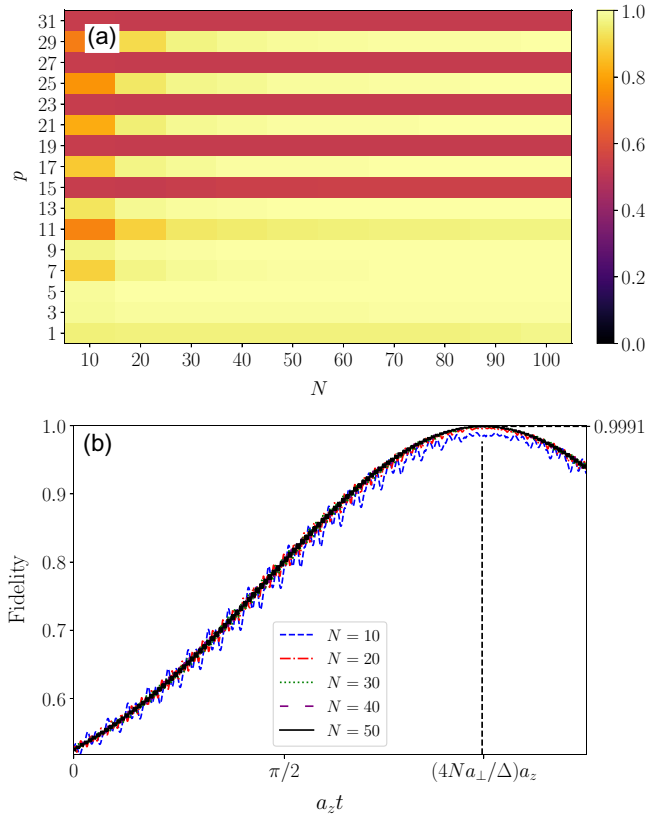


FIG. 4. (a) Maximum relative average gate fidelity for the Hadamard gate derived from the exact dynamic $\tilde{H}(t)$ according to Eq. (21), for various N and p , indicating the region where one can achieve a fidelity of around 0.99. (b) The first few instances for the case $p = 5$, where one can achieve fidelity 0.9991 for $N = 50$ at the evolution time $t = 4a_{\perp}N/\Delta = 20.21$ ns. The descriptions for the presentations are similar to those for Fig. 2.

leading to a maximum value only when $p - 1$ is divisible by 4. This oscillation appears merely as a global phase in the preparation of the X gate and thus remains unobservable.

Apart from that, even though the gate is prepared by the operator $\hat{U}_x$ as in the case of the X gate, a higher relative average gate fidelity can be observed here because the evolution period of $\hat{U}_x$ in this implementation is shorter, resulting in less accumulation of the extra terms removed in the approximation. Another contributing factor is the initialization of the electron spin, which acts as a projective operator and suppresses coherence propagation in the dynamics, leading to a reduced deformation in the observed fidelity.

Unlike the preparation of X and Z gates, these effects can contribute to a slightly larger deviation from the optimal time. In particular, we find that such deviations are bounded by $0.01223 a_z^{-1}$, which is, however, negligibly small.

V. GHZ-STATE PREPARATION

Apart from the collective gate implementation, it is possible to use the entangling gates Eqs. (10a) and (10b) for a different purpose, e.g., the preparation of nuclear-entangled states. In this section, we demonstrate this aspect by using them for the preparation of the GHZ state on a three-qubit subspace $\mathcal{H}_{\alpha\beta}$.

A. Initialization

First of all, we assume that one can perform initialization of the nuclear spin states in $|m_I\rangle^{\otimes 3}$ for $m_I = \pm 1$. This can be done via a combination of polarization to ground states and conditional rotation using our derived gates. For polarization to the ground state, e.g., the state $|-1\rangle^{\otimes 3}$, one can employ, for instance, a hyperpolarization procedure introduced in Ref. [56], where the electron spin is polarized and the flip-flop interaction is used. Another method, proposed in Ref. [55], involves the application of continuous optical pumping close to the level crossing, where the state $|0\rangle \otimes |1\rangle^{\otimes 3}$ can be initialized. Therefore, in the following discussion, we assume that the nuclear initial spin state is prepared in $|m_I\rangle^{\otimes 3}$ for $m_I = \pm 1$.

According to the notation adopted in Sec. III A, one has

$$|m_I\rangle_k = \frac{m_I|x\rangle_k + |y\rangle_k}{\sqrt{2}}. \quad (24)$$

As discussed earlier, the application of the unitary operators Eqs. (13a) or (13b) will keep one component unchanged while rotating the other component to another orthogonal state. For instance, we observe that

$$e^{\pm i\varphi \hat{I}_k^x} |m_I\rangle_k = \frac{m_I|x\rangle_k + \cos \varphi |y\rangle_k \pm i \sin \varphi |z\rangle_k}{\sqrt{2}},$$

and in particular for $\varphi = \pi/2$, this becomes

$$e^{\pm i(\pi/2) \hat{I}_k^x} |m_I\rangle_k = \frac{m_I|x\rangle_k \pm i|z\rangle_k}{\sqrt{2}}, \quad (25)$$

for $m_I = \pm 1$. This property can be exploited for the preparation of GHZ states.

B. Formulations

The GHZ state [64] of three qubits is written as

$$|\text{GHZ}\rangle_v = \frac{|\bar{0}\bar{0}\bar{0}\rangle + e^{iv} |\bar{1}\bar{1}\bar{1}\rangle}{\sqrt{2}}, \quad (26)$$

where the qubit k is described by some Hilbert space spanned by $\{|\bar{0}\rangle_k, |\bar{1}\rangle_k\}$ and v is an arbitrary phase. We now demonstrate as an example that one can use the entangling gate $\hat{U}_x(\pi/2)$ to prepare a GHZ state on a subspace zx of the three nuclear spins. This can be done through the

conditional rotation of Eq. (17b), where the nuclear spins are rotated in different directions for the different electron spin control states. Together with a preparation and a measurement of electron spin in a superposition state, which results in the superposition of the rotated states on the nuclear part, it can be seen that the nuclear reduced state for each measurement outcome will become the GHZ state.

In particular, from Eq. (25), let us define

$$|\bar{0}\rangle_k = e^{-i(\pi/2)\hat{I}_k^x} |m_I\rangle_k = \frac{m_I|x\rangle_k - i|z\rangle_k}{\sqrt{2}}, \quad (27)$$

$$|\bar{1}\rangle_k = e^{i(\pi/2)\hat{I}_k^x} |m_I\rangle_k = \frac{m_I|x\rangle_k + i|z\rangle_k}{\sqrt{2}}, \quad (28)$$

for each spin k . Note that $|\bar{0}\rangle_k$ and $|\bar{1}\rangle_k$ are orthonormal states, and additionally $\{|\bar{0}\rangle_k, |\bar{1}\rangle_k\}_k$ form a basis of the zx subspace. Let the state be initialized to $|0\rangle \otimes |m_I\rangle^{\otimes 3}$, as previously discussed. Since $|0\rangle = (|+\rangle + |-\rangle)/\sqrt{2}$, by applying the rotation gate, one gets

$$\hat{U}_x(\pi/2) |0\rangle \otimes |m_I\rangle^{\otimes 3} = \frac{|+\rangle \otimes |\bar{0}\bar{0}\bar{0}\rangle + |-\rangle \otimes |\bar{1}\bar{1}\bar{1}\rangle}{\sqrt{2}}. \quad (29)$$

Next, one can measure the central spin state with the basis $\{|0\rangle, |-1\rangle\}$, where the measurement results will herald the nuclear spin state. Namely, if the central spin state after the measurement is found to be $|0\rangle$, the nuclear spin will be left in the state $|\text{GHZ}\rangle_0$, whereas it will be $|\text{GHZ}\rangle_\pi$ if the electron spin is found at the state $|-1\rangle$.

Remarkably, if the mentioned measurement is realized by a projection onto the state $|0\rangle$ or $|-1\rangle$, the state of the nuclear spins is mapped to GHZ states in both successful and non-successful measurements, with different phases $\nu = 0$ and $\nu = \pi$, which can be heralded from the central spin measurement outcome. For the negative outcome branch, such a phase in $|\text{GHZ}\rangle_\pi$ can be corrected by further applying a postprocessing operation $\hat{U}_y(\pi/2)$, resulting in

$$\hat{U}_y(\pi/2) |-1\rangle \otimes |\text{GHZ}\rangle_\pi = (-i\hat{\sigma}_y |-1\rangle) \otimes |\text{GHZ}\rangle_0. \quad (30)$$

The relation above comes from the observation that $|\bar{0}\rangle_k \langle \bar{0}| - |\bar{1}\rangle_k \langle \bar{1}| = m_I \hat{Y}_k^x$, which can be prepared from $\hat{U}_y(\pi/2)$ in a similar fashion as for Eq. (18).

Indeed, the entangling gate $\hat{U}_x(\pi/2)$ with some postprocessing can be used to prepare GHZ states in the zx subspace. Such states can be further transferred to other collective subspaces by applying another rotation step. For example, one can write

$$\begin{aligned} \hat{U}_z(\pi/2) (|0\rangle \otimes |\text{GHZ}\rangle_\nu) &= |0\rangle \otimes \prod_k (\hat{P}_k^z - i\hat{X}_{xy}) |\text{GHZ}\rangle_\nu \\ &= |0\rangle \otimes |\widetilde{\text{GHZ}}\rangle_\nu, \end{aligned}$$

where $|\widetilde{\text{GHZ}}\rangle_\nu$ takes the same form as $|\text{GHZ}\rangle_\nu$ with the replacement of $|x\rangle_k$ by $-i|y\rangle_k$, i.e., the GHZ state in the yz subspace. We note that introducing this transformation will degrade the concerned fidelity; hence, if one expects operational qubits in the yz subspace, in practice, the overall fidelity including the effect of the transformation $\hat{U}_z(\pi/2)$ should be taken into account.

The procedure for GHZ-state preparation can be generalized to the writing process on the nuclear spin collective qubit. For instance, using $\{|\bar{0}\bar{0}\bar{0}\rangle, |\bar{1}\bar{1}\bar{1}\rangle\}$ as a basis for the nuclear collective qubit, and replacing the electron spin state $|0\rangle$ on the left-hand side of Eq. (29) by $\alpha|+\rangle + \beta|-\rangle$, the coefficients in the resulting nuclear spin collective states after measurement of the electron spin in the $\{|0\rangle, |-1\rangle\}$ basis will be $\alpha|\bar{0}\bar{0}\bar{0}\rangle \pm \beta|\bar{1}\bar{1}\bar{1}\rangle$, where the sign depends on the measurement outcome. For the reading process, one could employ the same entangling gates to conditionally transfer the nuclear spin collective state to the electron spin state. For example, one can see that $\hat{U}_z(\pi/12)\hat{U}_x(\pi/2)|0\rangle \otimes (\alpha|\bar{0}\bar{0}\bar{0}\rangle \pm \beta|\bar{1}\bar{1}\bar{1}\rangle) = (\tilde{\alpha}|0\rangle - im_I\tilde{\beta}|1\rangle) \otimes |\xi\rangle$, where $\tilde{\alpha} = (\alpha + \beta)/\sqrt{2}$ and $\tilde{\beta} = (\alpha - \beta)/\sqrt{2}$, while $|\xi\rangle$ is an irrelevant nuclear spin collective state. This suggests that the synchronous gates allow us to use the three nuclear spins as a collective qubit whose manipulation can be achieved via the electron spin mediator.

C. Fidelity of the GHZ-state preparation

Here, we numerically demonstrate the fidelity in the preparation of GHZ states by our protocol. We set the initial state as $|\psi_0\rangle = |0\rangle \otimes |1\rangle^{\otimes 3}$, and, for simplicity, we assume short and perfect Pauli gates $\hat{\sigma}_z$ and $\hat{\sigma}_x$ (and also their corresponding Hadamard gates) for the electron spin. For the mixed state, we use the state fidelity defined as [65]

$$F(\rho, \sigma) = \text{Tr} \left(\sqrt{\sqrt{\sigma} \rho \sqrt{\sigma}} \right) \quad (31)$$

between the outcome states from our protocol and the target GHZ states. We compute the fidelity between $|\text{GHZ}\rangle_{0,\pi}$ and the nuclear spin state

$$\rho_+(t) = \text{Tr}_{cs} \left[(|0\rangle\langle 0| \otimes \mathbb{1}) \hat{U}_z(t) |\psi_0\rangle\langle \psi_0| \hat{U}_z^\dagger(t) \right], \quad (32a)$$

$$\rho_-(t) = \text{Tr}_{cs} \left[(|-1\rangle\langle -1| \otimes \mathbb{1}) \hat{U}_z(t) |\psi_0\rangle\langle \psi_0| \hat{U}_z^\dagger(t) \right], \quad (32b)$$

where Tr_{cs} is the partial trace over the central spin qubit. We write

$$F_\nu^\pm(t) = F(\rho_\pm(t), \rho_\nu^{\text{GHZ}}),$$

where $\rho_\nu^{\text{GHZ}} = |\text{GHZ}\rangle_\nu \langle \text{GHZ}|$, for the fidelity at time t for the considered pair of states.

In Fig. 5, the fidelity $F_v^\pm(t)$ is illustrated with the same parameters given for the preparation of the X gate. One can see that our protocol can produce GHZ states with a fidelity greater than 0.99. As we discussed for the fidelity of the Hadamard gate, the fidelity in this case is larger than the protocol for the preparation of $\hat{X}_{yz}$, with both initialization and measurement operators here being projective, leading to a removal of interference effects. The fidelity can become distorted when Δ is not sufficiently large, for instance, when $B = 169$ mT ($N = 10$). At a sufficiently large field, e.g., $B = 345$ mT ($N = 50$), our approximation of the entangling gate works well and can be employed for the preparation of the GHZ states as expected. For $\nu = 0$, the fidelity is 0.9985 at the optimal time and 0.9963 at $t = 4Na_\perp/\Delta$, while for $\nu = \pi$, the fidelity is 0.9984 at the optimal time and 0.9955 at $t = 4Na_\perp/\Delta$. We observe larger deviations in optimal times from the referent value $t = 4Na_\perp/\Delta$ compared to the preparation of the X gate, i.e., $0.1055 a_z^{-1}$ for $\nu = 0$ and $0.1651 a_z^{-1}$ for $\nu = \pi$. In practice, without additional information, there is no instructive method to determine the optimal time, and one can only expect the gate at the time $t = 4Na_\perp/\Delta$, i.e., at the time of completion of N cycles of the control pulse sequence. Hence, in realistic implementation, this deviation should always be taken into account. Nonetheless, thanks to the slow changes around the optimal point, the fidelities observed at $t = 4Na_\perp/\Delta = 40.43$ ns can be large, exceeding 0.99, as reported above. The total preparation time of the GHZ states, including the reinitialization Eq. (25), which is done by the X gate, will then be about 80.85 ns.

VI. ELECTRON SPIN DEPHASING

We have discussed the gates and GHZ state implications under perfect conditions, where each nuclear spin interacts only with the central spin, and the whole cluster is isolated from the external bath. In this section, we will demonstrate the contribution of electron spin dephasing to the obtained fidelities. The dephasing can arise from hyperfine interactions with the nuclear spin bath and thermal phonons [37,66,67]. This effect may also result from deformation of the host material, which per se can also be employed to extend the coherence time [68]. One can also expect that impurities or imperfections of the sample might contribute to the coherence time, as suggested for NV centers in diamond [69–72] and color centers in SiC [73]; however, studies of this aspect are still open for the hBN system.

The dephasing can be modeled by a dissipative generator in the Lindblad equation for the whole system density matrix ρ , i.e.,

$$\frac{d\rho}{dt} = -i[\tilde{H}(t), \rho] + \frac{\Gamma}{2} \left(2\hat{L}\rho\hat{L}^\dagger - \hat{L}^\dagger\hat{L}\rho - \rho\hat{L}^\dagger\hat{L} \right), \quad (33)$$

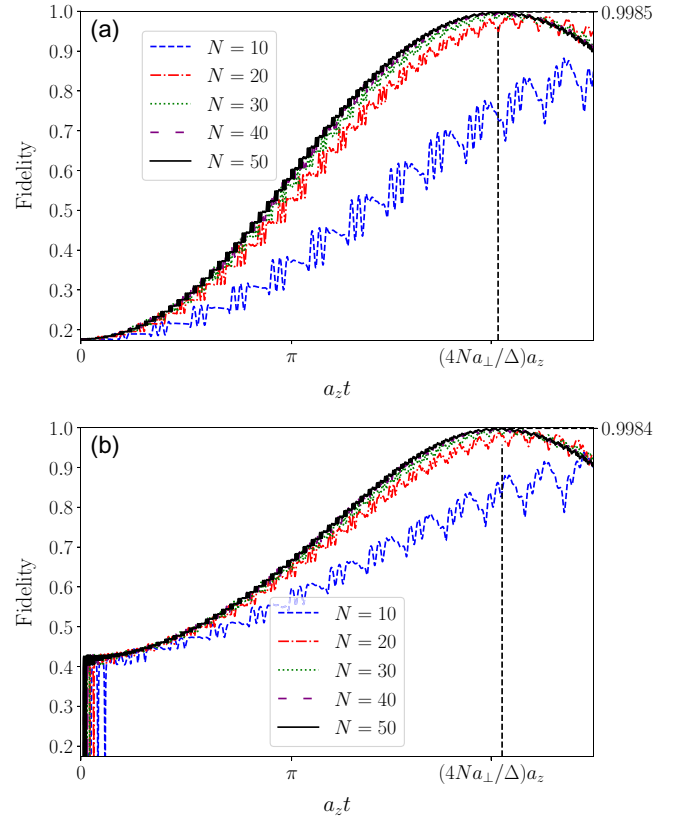


FIG. 5. (a) Fidelity of the nuclear spin state after the operation Eqs. (32a) and (32b) on $|\psi_0\rangle = |0\rangle \otimes |1\rangle^{\otimes 3}$ for a measurement result $|0\rangle$ with respect to the GHZ state $|\text{GHZ}\rangle_0$, with various numbers of revolutions N and with $p = 5$. (b) Similar results for the negative measurement result $|-1\rangle$ with the referent state $|\text{GHZ}\rangle_\pi$. Note that the operational magnetic field strengths are given by the expression Eq. (23). For both cases, unlike the gate fidelities, one can observe slight deviations of the optimal times (vertical dashed lines) from the predicted value $t = 4Na_\perp/\Delta = 40.43$ ns.

where $\hat{L} = \hat{\sigma}_x \otimes \mathbb{I}$ defines a dephasing generator in the concerned two-level electron spin subspace and $\Gamma > 0$ is the pure dephasing rate of the electron spin. The experimentally reported dephasing time depends on temperature. At room temperature, its typical value is around $\Gamma^{-1} \sim 2 \mu\text{s}$ and can be larger at lower temperature; see, e.g., Refs. [32,74]. Here, we set $\Gamma^{-1} = 2 \mu\text{s}$ for the room-temperature value and $4 \mu\text{s}$ at a lower temperature in our illustration. Another factor that may degrade the fidelity of the gates or prepared GHZ states is the electric quadrupole interaction of the nuclear spins, which modifies Eq. (2) to $\hat{H}_n = \sum_k -\gamma_k \mathbf{B} \cdot \mathbf{I}_k + Q_k (\hat{I}_k^z)^2$ with $Q_k \approx 0.383 \cdot 2\pi \times \text{MHz}$ according to experimental observations [32]. We have also included this interaction in our numerical considerations and found that the effect is negligibly small and does not appreciably affect the gate and state fidelities. In particular, the relative deviations (defined below) caused by the quadrupole interaction are less than 0.25%

for the gate fidelities and are limited to 0.015% for the state fidelities.

To determine the effects of noise, we consider a relative deviation defined by

$$\varepsilon = \frac{F_{\text{ref}} - F_{\text{noise}}}{F_{\text{ref}}}, \quad (34)$$

where F_{ref} refers to the reference fidelity and F_{noise} is the fidelity including the noisy contribution mentioned above. The reference fidelities are the same as those computed in the previous section for gates and states, while F_{noise} includes dephasing effects in the dynamics. For illustration, for the X gate, H gate, and GHZ states, we set $N = 50$ and $p = 5$, with magnetic field strengths calculated using Eq. (23), while for the Z gate, the magnetic field strength is $B = 500$ mT. For simplicity, we compute the relative deviations at $t = \pi a_z^{-1}$ for the Z gate, and $t = 4a_{\perp}N/\Delta$ for the X gate, Hadamard gate, and GHZ states. We note that, as previously discussed, these times are not the exact optimal times for the evolution $\hat{H}$, but they are close to the optimal times relative to the time scale a_z^{-1} . In Fig. 6(a), the relative deviations for the X , Z , and Hadamard H gates are shown, where decreases in deviations are seen for longer coherence times, i.e., lower temperatures. All observed deviations range from a few to several percent, which can be mitigated by further optimization, e.g., modifying the filter functions $F_{\alpha}(t)$. This suggests that our protocols for gate implementation are noise resilient.

In addition, we observe that the implementation of the X gate suffers the most deviation: 1.64% for $\Gamma^{-1} = 2 \mu\text{s}$ and 0.83% for $\Gamma^{-1} = 4 \mu\text{s}$. This agrees with the fact that the evolution time required for its implementation is the longest, e.g., $6.116 a_z^{-1} = 40.43$ ns in our illustrations, compared to $\pi a_z^{-1} = 20.76$ ns for the implementation of the Z gate. For the Hadamard gate H , one can see the least deviation from the expected value. This can be explained by the initialization of the electron spin in our protocol, which limits the sample region in the calculation of average gate fidelity. This removes some correlation propagation in the dynamics from the expected value, leading to higher fidelity as well as lower deviation from the noisy terms in general; however, as in typical schemes involving projective operators, including initialization or postselection processes, a higher fidelity can usually be compensated by a lower success probability, i.e., the success probability for the electron spin initialization in our case.

A similar deviation can be observed for the GHZ-state preparation in Fig. 6(b). The asymmetric nature of the deformation from the dephasing term for the states $|\text{GHZ}\rangle_0$ and $|\text{GHZ}\rangle_{\pi}$ can also be seen. Although the mechanism for the preparation is similar to the implementation of the X gate, we see that the fidelity suffers less deviation

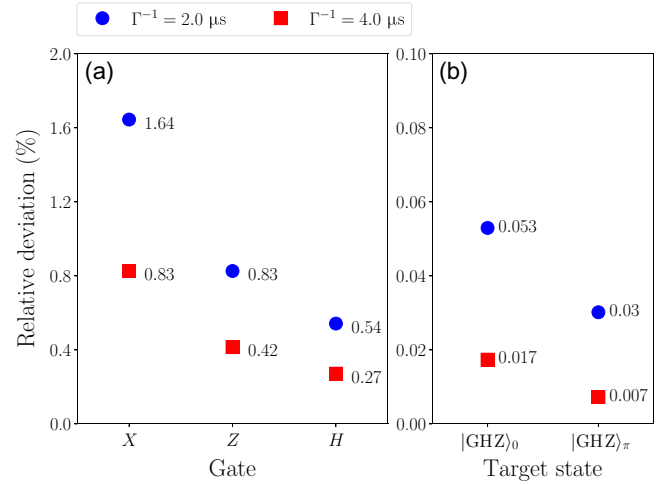


FIG. 6. (a) Relative deviations of the fidelity for gate implementations. (b) Relative deviations of the fidelity for GHZ-state preparation. We use $B = 500$ mT for the calculation of the Z gate, where $N = 50$ and $p = 5$ are employed in the calculation for the X gate, H gate, and GHZ states. The deviation for implementing the X gate is larger than the other two due to the longer evolution time of $\hat{U}_x$, while the implementation of the H gate benefits from a deviation discount from the initialization in the protocol. From both gate fidelities and state fidelities, it is seen that the longer coherence time, achievable below room temperature, leads to smaller deviations in the fidelity profiles.

from the noisy terms. This is because, unlike gate fidelity, the initial state and the measurement are predetermined. On one hand, there is no accumulation of deviation from the sampling process over the state space in the calculation of the fidelity, as in the case of average gate fidelity. On the other hand, similar to the implementation of the Hadamard gate, the projective characteristic of the measurement also removes coherence in the dynamics from the obtained quantity.

VII. CONCLUSIONS

To summarize, we have derived a set of entangling gates on three ^{14}N nitrogen nuclear spins through a VB center in hBN, using the electron spin of the defect as a control qubit. Such gates are attained by imposing a strong enough magnetic field along the VB center axis of symmetry, i.e., perpendicular to the lattice plane, where the $\hat{U}_z$ gate can be obtained by removal of fast oscillation terms and $\hat{U}_x$ can be achieved by the application of control pulses. We employ the derived unitary rotations to implement the synchronous three-qubit Pauli X gate and Z gate, as well as the Hadamard gate on some relevant three-qubit subspace. Using a set of realistic system parameters taken from computational and experimental works, we have demonstrated numerically that such gates can be obtained with high fidelities. This suggests that our scheme is a promising protocol for gate implementation upon nuclei in hBN,

implementable in future experiments. We further use the entangling gates to prepare GHZ states, where a fidelity above 0.99 can be observed numerically. Finally, we consider the effect of electron dephasing, where the relative deviations of the gate fidelities from the noisy terms are less than 2%, and even less than 0.1% for the preparation of GHZ states. These results suggest that our protocols for the synchronous three-qubit gates and the preparation of GHZ states are noise resilient and thus promising for experimental realizations and potentially for quantum computing applications. In addition, given the possibility to control several qubits at once with the synchronous gate, these are also interesting protocols for fault-tolerance applications on a realistic platform.

With the implementation of the synchronous gates and the preparation of the GHZ states, our work can be treated as the first step in exploiting the utility of a nuclear spin cluster around a VB center in hBN as a platform for quantum computation. On one end, one can further explore the use of the entangling gates for the implementation of different gates, as well as two-qubit-like gates, which will lead to a complete set of universal gates. On the other end, one can also consider different parameters, e.g., magnetic field and control field, as well as other time scales, to execute different parts of the system dynamics, allowing for the implementation of single-nuclear-spin qubit gates or large-scale information processing. The research in this direction, in our belief, is a promising area that can enable V_B^- -hBN as a candidate for a quantum computational platform in general. It is worth mentioning that, thanks to recent advances in preparing highly isotopically purified samples, the investigations performed in this work can even be extended to the case of spin-1/2 clusters of ^{15}N nuclei [30]. Finally, we should add that the rather large magnetic fields (~ 0.5 T) required for the validity of the rotating-wave approximation are currently available in labs; see, e.g., Ref. [57]. Nevertheless, this requirement partly limits the portability of a device operating based on our proposed protocol, since such magnetic field values can only be prepared in a stationary manner.

Several interesting approaches can improve our proposed protocols. The first of these is pulse optimization. We have used CPMG pulse sequences for the preparation of $\hat{U}_x$. This is one of the simplest schemes employed to minimize the unwanted terms in the Hamiltonian to arrive at a workable approximation. This can be replaced by more advanced pulse sequences, where one can prepare in a more optimal fashion. Namely, one can construct a pulse sequence for which the filter functions $F_\alpha(t)$ minimize the contribution from $\hat{H}_{\text{RW,odd}}$ and $\hat{H}_{\text{CRW}}$, e.g., by minimizing $\|\hat{H}_{\text{RW,odd}} + \hat{H}_{\text{CRW}}\|_{\text{op}}$, where $\|\cdot\|_{\text{op}}$ is an operator trace norm. Another aspect is the extension of the gate implementation to gates beyond Pauli and rotation gates. In our

examples of the X and Z gates, unlike the preparation of GHZ states, the electron spin does not play a significant role as a control qubit. It is then interesting to examine whether one can use the control qubit and prepare an effective two-qubit gate (e.g., electron qubit and any of the nuclear qubits) based on a similar mechanism and possibly construct a complete universal set of gates on the qubit systems.

Apart from using dynamical decoupling pulses for gate implementation, one can also use microwave or rf pulses to control and manipulate nuclear spins [75]. Furthermore, one can combine dynamical decoupling pulses with microwave or rf pulses to engineer optimally desired gates with high fidelity [17,27,29]. In particular, instead of defining a computational basis from the free Hamiltonian and exploiting the interaction terms as gate actions, one can use the full Hamiltonian, including the interaction, to define a computational basis and address the transitions of the gate actions by microwave or rf pulses. These techniques require more complex control schemes compared to our protocol to achieve the desired operations, and they can also lead to longer operation times when a considerable number of microwave or rf pulses are required. The latter makes those techniques more demanding when coherence and relaxation times are taken into account; however, they have the advantage of greater flexibility for nuclear spin manipulation. Full investigation of this technique is out of the scope of this work and is the subject of future work.

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DATA AVAILABILITY

The data that support the findings of this article are openly available [76].

APPENDIX A: ROTATED HAMILTONIAN

Here, we derive the expression of the rotated Hamiltonian, Eq. (7) in the main text. Following the conditions we supposed in the main text, the Hamiltonian Eq. (5) in the rotating frame for the free Hamiltonian

$$\hat{H}_0 = -\frac{\omega_0 \hat{\sigma}_z}{2} - \sum_k \omega_k \hat{I}_k^z + \hat{H}_C(t) \quad (\text{A1})$$

can be written in the following form:

$$\begin{aligned}
\tilde{H}(t) = & F_z(t) \sum_k \left(\frac{A_k^{zz}}{2} \right) \hat{\sigma}_z \hat{I}_k^z \\
& + \sum_k A_k^\perp \cos \Delta_k t \left(F_x(t) \hat{\sigma}_x \hat{I}_k^x + F_y(t) \hat{\sigma}_y \hat{I}_k^y \right) \\
& - \sum_k A_k^\perp \sin \Delta_k t \left(F_x(t) \hat{\sigma}_x \hat{I}_k^y - F_y(t) \hat{\sigma}_y \hat{I}_k^x \right) \\
& + \sum_k B_k^\perp \cos \Sigma_k t \left(F_x(t) \hat{\sigma}_x \hat{I}_k^x - F_y(t) \hat{\sigma}_y \hat{I}_k^y \right) \\
& + \sum_k B_k^\perp \sin \Sigma_k t \left(F_x(t) \hat{\sigma}_x \hat{I}_k^y + F_y(t) \hat{\sigma}_y \hat{I}_k^x \right) \\
& - \sum_k \left(\frac{A_k^{xy}}{2\sqrt{2}} \right) \sin \Sigma_k t \left(F_x(t) \hat{\sigma}_x \hat{I}_k^x - F_y(t) \hat{\sigma}_y \hat{I}_k^y \right) \\
& + \sum_k \left(\frac{A_k^{xy}}{2\sqrt{2}} \right) \cos \Sigma_k t \left(F_x(t) \hat{\sigma}_x \hat{I}_k^y + F_y(t) \hat{\sigma}_y \hat{I}_k^x \right),
\end{aligned} \tag{A2}$$

where we write $\Delta_k = \omega_0 - \omega_k$ and $\Sigma_k = \omega_0 + \omega_k$ as the rotating-wave and counter-rotating-wave frequencies for the nuclear spin k , respectively, and $A_k^\perp = (A_k^{xx} + A_k^{yy})/2\sqrt{2}$ and $B_k^\perp = (A_k^{xx} - A_k^{yy})/2\sqrt{2}$.

Let us use the parameters for $\mathbb{A}_k$ from Ref. [55]:

$$\mathbb{A}_1 = \begin{pmatrix} 79.406 & 18.391 & 0 \\ 18.391 & 58.170 & 0 \\ 0 & 0 & 48.159 \end{pmatrix}, \tag{A3}$$

$$\mathbb{A}_2 = \begin{pmatrix} 46.944 & 0 & 0 \\ 0 & 90.025 & 0 \\ 0 & 0 & 48.158 \end{pmatrix}, \tag{A4}$$

$$\mathbb{A}_3 = \begin{pmatrix} 79.406 & -18.391 & 0 \\ -18.391 & 58.170 & 0 \\ 0 & 0 & 48.159 \end{pmatrix}, \tag{A5}$$

where the elements are expressed in units of $2\pi \times \text{MHz}$. With these parameters, it is observed that several parameters are approximately uniform for all nuclear spins, namely A_k^{zz} and the sum of the in-plane diagonal terms $A_k^{xx} + A_k^{yy}$. Since $\omega_k = \gamma_n B + A_k^{zz}/2$, it is then possible to replace the rotating frequencies Δ_k with their average $\Delta = \sum_k (\omega_0 - \omega_k)/3$. Likewise, one can use the scaled averages

$$a_z = \frac{1}{6} \sum_k A_k^{zz}, \quad a_\perp = \frac{1}{6\sqrt{2}} \sum_k (A_k^{xx} + A_k^{yy})$$

in place of the coefficients in the rotating terms. Finally, to achieve the expression in Eq. (7),

$$\begin{aligned}
\tilde{H}(t) \approx & a_z F_z(t) \hat{\sigma}_z \sum_k \hat{I}_k^z + a_\perp F_x(t) \cos \Delta t \hat{\sigma}_x \sum_k \hat{I}_k^x \\
& + a_\perp F_y(t) \cos \Delta t \hat{\sigma}_y \sum_k \hat{I}_k^y \\
& + \hat{H}_{\text{RW, odd}}(t) + \hat{H}_{\text{CRW}}(t),
\end{aligned}$$

we write

$$\hat{H}_{\text{RW, odd}}(t) = - \sum_k A_k^\perp \sin \Delta_k t \left(F_x(t) \hat{\sigma}_x \hat{I}_k^y - F_y(t) \hat{\sigma}_y \hat{I}_k^x \right),$$

and write $\hat{H}_{\text{CRW}}(t)$ to represent all the counter-rotating terms in Eq. (A2), i.e., all the terms associated with frequencies Σ_k .

APPENDIX B: INSERTION OF MULTIPLE FILTER FUNCTIONS

To simplify the problem, let us consider the cluster Hamiltonian in the form

$$\tilde{H}_1(t) = \sum_{\alpha=x,y,z} \hat{\sigma}_\alpha \hat{H}_\alpha(t) + \hat{H}_C(t), \tag{B1}$$

where $\hat{H}_C(t)$ is the control field. In our setup, the first term is simply the expression in Eq. (5) in the rotating frame with respect to the free Hamiltonian Eq. (A1) without the control term, or it can even be the Hamiltonian in the tilted frame in the main line consideration. Here, we write the local control field $\hat{H}_C(t)$ as

$$\begin{aligned}
\hat{H}_C(t) = & h_z(t) \hat{\sigma}_z + h_x(t) \hat{\sigma}_x + h_y(t) \hat{\sigma}_y \\
= & \mathbf{h}(t) \cdot \boldsymbol{\sigma} = h(t) \hat{\mathbf{h}}(t) \cdot \boldsymbol{\sigma},
\end{aligned} \tag{B2}$$

where the first term is the added variation of the magnetic field and the remaining term corresponds to the microwave field driving the transfer between two levels.

Transform the Hamiltonian Eq. (B1) into the rotating frame for the control Hamiltonian $\hat{H}_C(t)$. It follows that

$$\tilde{H}(t) = \sum_{\alpha=x,y,z} \hat{\sigma}_\alpha(t) \hat{H}_\alpha(t), \tag{B3}$$

where $\hat{\sigma}_\alpha(t) = \mathcal{T} e^{i \int_0^t dt' \hat{H}_C(t')} \hat{\sigma}_\alpha \overline{\mathcal{T}} e^{-i \int_0^t dt' \hat{H}_C(t')}$, and $\mathcal{T}$ and $\overline{\mathcal{T}}$ are the time-ordering (the leftmost is the first event) and time-antioordering operators (the leftmost is the last event), respectively.

In dynamical decoupling, apart from the oscillating current, the simplest and most employed type of control

functions $h_\alpha(t)$ are square pulses. In particular, we suppose that

$$\begin{aligned} \mathbf{h}(t) &= \sum_{\ell=1}^n [\Theta(t_\ell) - \Theta(t_{\ell-1})] \mathbf{h}_\ell \\ &= \sum_{\ell=1}^n [\Theta(t_\ell) - \Theta(t_{\ell-1})] h_\ell \hat{\mathbf{h}}_\ell \cdot \boldsymbol{\sigma}, \end{aligned}$$

where $\mathbf{h}_\ell$ are constant vectors, $0 = t_0 \leq t_1 \leq \dots \leq t_n$, and

$$\Theta(t) = \begin{cases} 1, & t \geq 0 \\ 0, & \text{otherwise} \end{cases}$$

is a Heaviside function. Let $\hat{\sigma}_\ell = \hat{\mathbf{h}}_\ell \cdot \boldsymbol{\sigma}$ and $\tau_\ell = t_\ell - t_{\ell-1}$. Thus,

$$\begin{aligned} \mathcal{T} e^{i \int_0^t dt \hat{H}_C(t)} &= \prod_{\ell=1}^n e^{i \tau_\ell h_\ell \hat{\sigma}_\ell} \\ &= \prod_{\ell=1}^n [\mathbb{1} \cos(h_\ell \tau_\ell) + i \hat{\sigma}_\ell \sin(h_\ell \tau_\ell)], \end{aligned}$$

and then

$$\hat{\sigma}_\alpha(t) = T_{h_1 \tau_1, \sigma_1} \circ \dots \circ T_{h_n \tau_n, \sigma_n} [\hat{\sigma}_\alpha], \quad (\text{B4})$$

where

$$\begin{aligned} T_{h_\ell \tau_\ell, \hat{\sigma}_\ell} [\hat{\sigma}_\alpha] &= \hat{\sigma}_\alpha \cos^2(h_\ell \tau_\ell) + (\hat{\sigma}_\ell \hat{\sigma}_\alpha \hat{\sigma}_\ell) \sin^2(h_\ell \tau_\ell) \\ &\quad + i [\hat{\sigma}_\ell, \hat{\sigma}_\alpha] \frac{\sin(2h_\ell \tau_\ell)}{2}. \end{aligned} \quad (\text{B5})$$

The last term in Eq. (B5) is the crucial term providing a drift from the operator $\hat{\sigma}_\alpha$. This term can be eliminated by setting $h_\ell \tau_\ell = \pi/2$ for all ℓ , and then $T_{\pi/2, \hat{\sigma}_\ell} [\hat{\sigma}_\alpha] = \hat{\sigma}_\ell \hat{\sigma}_\alpha \hat{\sigma}_\ell$. Choosing $\hat{\sigma}_\ell$ from the set $\{\mathbb{1}, \hat{\sigma}_x, \hat{\sigma}_y, \hat{\sigma}_z\}$ (where $\mathbb{1}$ stands for $h_\ell = 0$ during that time interval), it follows that

$$\hat{\sigma}_\alpha(t) = \left[\prod_{\ell=1}^n \hat{\sigma}_\ell \right] \hat{\sigma}_\alpha \left[\prod_{\ell=n}^1 \hat{\sigma}_\ell \right] = F_\alpha(t) \hat{\sigma}_\alpha, \quad (\text{B6})$$

where $F_\alpha(t)$ is the filter function defined by

$$F_\alpha(t) = (-1)^{\sum_\ell (1 - \delta_{\alpha\ell}) (1 - \delta_{\alpha\ell} 0)}, \quad (\text{B7})$$

and $\alpha_\ell = 0, x, y, z$ corresponds to the choice of the control operator on the interval $(t_{\ell-1}, t_\ell)$.

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