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# Band-selective shaped pulse for high fidelity quantum control in diamond

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High fidelity quantum control of qubits is crucially important for realistic quantum computing, and it becomes more challenging when there are inevitable interactions between qubits. We introduce a band-selective shaped pulse, refocusing BURP (REBURP) pulse, to cope with the problems. The electron spin of nitrogen-vacancy centers in diamond is flipped with high fidelity by the REBURP pulse. In contrast with traditional rectangular pulses, the shaped pulse has almost equal excitation effect in a sharply edged region (in frequency domain). So the three sublevels of host <sup>14</sup>N nuclear spin can be flipped accurately simultaneously, while unwanted excitations of other sublevels (e.g., of a nearby <sup>13</sup>C nuclear spin) is well suppressed. Our scheme can be used for various applications such as quantum metrology, quantum sensing, and quantum information process. © 2014 AIP Publishing LLC. [<http://dx.doi.org/10.1063/1.4885772>]

Coherent manipulation of high fidelity is a fundamental prerequisite for many applications such as quantum information process (QIP), quantum metrology, and quantum sensing. In actual quantum computing, precise quantum gates are required to satisfy the DiVincenzo criteria.<sup>1</sup> Scalable QIP requires more qubits with coherent interaction.<sup>2–4</sup> For local control gates, every qubit needs to be addressed accurately and controlled separately.<sup>5</sup> In principle, each qubit can be distinguished by its different spatial location<sup>6</sup> or resonant frequency.<sup>7</sup> However, the controlling field (for example, microwave (MW)) usually cannot be focused on certain qubit without disturbing others.<sup>8</sup> Precise control of individual qubit becomes challenging. As a result, many techniques have been developed to optimize the quantum control fidelity such as gradient ascent pulse engineering (GRAPE) algorithm<sup>9</sup> and shaped pulse<sup>10</sup>

Shaped pulse is a technique using specially tailored pulses to suppress the effects caused by unwanted interaction and off-resonant excitation.<sup>11</sup> Both amplitudes and phases of the pulse sequences can be modulated according to numerical optimization or analytical approach to achieve an ideal quantum operation. Various pulse shapes, such as the Gaussian shape,<sup>12</sup> the Hermite shape,<sup>13</sup> and the band-selective, uniform response, pure-phase (BURP) family,<sup>14</sup> have been elaborately designed for diverse applications. Due to their outstanding properties, such as frequency selectivity,<sup>14</sup> self-refocusing behavior,<sup>15</sup> experimental robustness, and universality, these shaped pulses have been used in various physical systems, for example, nuclear magnetic resonance (NMR) systems<sup>16,17</sup> and laser spectroscopy.<sup>18,19</sup>

Spin or pseudospin qubits in solid state systems, such as quantum dots<sup>20</sup> and superconductor circuits,<sup>21</sup> are promising candidates for QIP. Among these, nitrogen-vacancy (NV)

center, which consists of a substitutional nitrogen atom next to a vacancy in the diamond lattice (depicted in Fig. 1(a)) has drawn much attentions these years.<sup>8,22–26</sup> By hyperfine interactions, NV electron spin with nuclear (ambient <sup>13</sup>C or host N) spins<sup>26</sup> or contiguous electron spins<sup>24</sup> can serve as multi-qubit system. However, as the number of qubits increases, optically detected magnetic resonance (ODMR) (Ref. 27) spectra become dense.<sup>8</sup> The unwanted interactions<sup>28</sup> and off-resonant excitation<sup>29,30</sup> block selectively high-fidelity control over individual qubit. Different techniques have been used to cope with these problems.<sup>8,31,32</sup> In this paper, we introduce another technique, refocusing BURP (REBURP) pulse, to optimize the control fidelity in NV system.

Our experiments are implemented with a single NV center in pure diamond (nitrogen concentration <5 ppb). With electron spin degeneracy of  $m_s = \pm 1$  lifted by external magnetic field  $\mathbf{B}$ , the Hamiltonian of a negative charged NV center (NV<sup>-</sup>) can be written as:<sup>33</sup>  $H = \Delta S_z^2 - \gamma_e \mathbf{B} \cdot \mathbf{S} - \gamma_N \mathbf{B} \cdot \mathbf{I}^{(N)} + A_{\parallel}^{(N)} S_z I_z^{(N)} + A_{\perp}^{(N)} (S_x I_x^{(N)} + S_y I_y^{(N)}) + P[(I_z^{(N)})^2 - \frac{1}{3}(\mathbf{I}^{(N)})^2]$

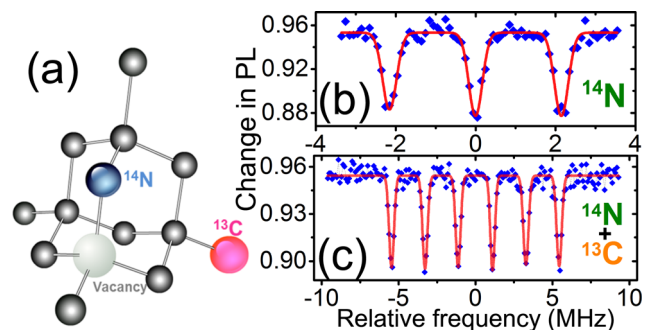


FIG. 1. The structure and different ODMR spectra of NV center. (a) The structure of a single NV center in diamond. (b) ODMR spectra of the NV center only with the host <sup>14</sup>N nucleus. (c) ODMR spectra of the NV center with a <sup>13</sup>C nucleus nearby.

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$-\gamma_C \mathbf{B} \cdot \sum_i \mathbf{I}_i^{(C)} + S_z \sum_i \mathbf{A}_i \cdot \mathbf{I}_i^{(C)}$ , where  $\Delta = 2.87 \text{ GHz}$  is the zero-field splitting of the ground state.  $\mathbf{S}$ ,  $\mathbf{I}_i^{(C)}$ ,  $\mathbf{I}_i^{(N)}$  are electron spin,  $^{13}\text{C}$ ,  $^{14}\text{N}$  nuclear spins;  $\gamma_e$ ,  $\gamma_C$ ,  $\gamma_N$  are the gyromagnetic ratios of them.  $A_{\parallel}^{(N)}$ ,  $A_{\perp}^{(N)}$ ,  $\mathbf{A}_i$  are the hyperfine interaction tensors for  $^{13}\text{C}$ ,  $^{14}\text{N}$  nuclear spins, and  $P$  is quadrupole coupling tensor. The ODMR spectra ( $m_s = 0 \leftrightarrow m_s = -1$ ) of a pure NV center without adjacent  $^{13}\text{C}$  nuclei are shown in Fig. 1(b), and the 3 dips induced by the hyperfine interaction with host  $^{14}\text{N}$  nuclear spin ( $I^N = 1$ ). When there is an adjacent  $^{13}\text{C}$  nuclear spin, as shown in Fig. 1(c), the hyperfine interaction with this spin 1/2 nucleus splits the 3 dips into 6 dips.<sup>34</sup> If more  $^{13}\text{C}$  nuclear spins are involved, the energy structure of the multi-qubit system will become more complicated and harder to control.

A home-built confocal microscope system, with MW components, is used to initialize, manipulate, and readout the spin states of the NV center at room temperature. To enhance the photon collection efficiency, a solid immersion lens (SIL) (Ref. 35) is etched above an NV center. After being amplified, the MW pulses used to manipulate the NV spin are delivered to the NV center through a coplanar waveguide (CPW) which is deposited close to the SIL.

The profile (time domain) of rectangular MW pulse, which is employed to manipulate the NV spin as a traditional technique, is shown in Fig. 2(a). The manipulating process can be described by Rabi oscillation<sup>29</sup> with Maxwell-Bloch equation as  $\omega(t) = \omega(0) \times \left\{ 1 + \left( \frac{\Omega'}{\Omega} \right)^2 \times [\cos(\Omega t) - 1] \right\}$ , where  $\Omega'$  is proportional to the square root of microwave power and  $\Omega = \sqrt{\Omega'^2 + \Delta^2}$  ( $\Delta$  is the frequency detuning). Both resonant and off-resonant excitation arises during the manipulations.<sup>30</sup> Furthermore, there are other frequency elements besides the carrier frequency in frequency domain. As shown in Fig. 2(b), when driving the NV spin with rectangular pulse, the response spectra in frequency domain are wide broadened and complicated. When several transitions are required for a simultaneous manipulation, detunings for some of them appear. As a result, the amplitude of Rabi oscillation will decrease, and the frequency will be asynchronous. Manipulations become imperfect and the fidelity decreases drastically. Though an increasing of the microwave power is useful under certain circumstances, it may disturb other states which need to be protected.<sup>36</sup>

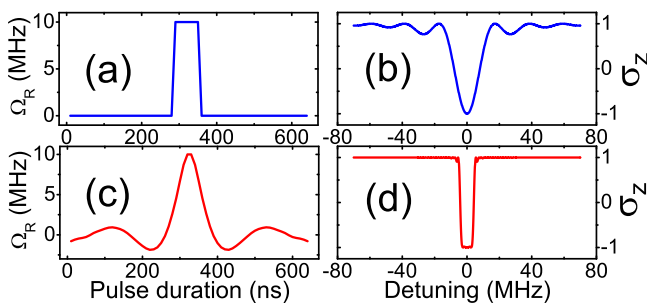


FIG. 2. Profile and spin response of the rectangular and shaped pulse. (a) A rectangular pulse in time domain. (b) Spin response (frequency domain) spectra of rectangular  $\pi$  pulse. (c) The profile (time domain) of REBURP shaped pulse. (d) Spin response (frequency domain) of the REBURP pulse.

To overcome the problems mentioned above, REBURP pulse is introduced, and its profile (in time domain) is displayed in Fig. 2(c). It is designed by simulated annealing method and standard gradient-descent routine.<sup>14,16</sup> As one kind of BURP pulses, REBURP pulse is band-selective, uniform response, pure-phase, and easy to implement in experiment. With band-selective property, it can get nearly perfect quantum operations within prescribed frequency range and suppress excitations beyond that region. Because of its uniform response, the operating efficiency of REBURP pulse does not rely on the initial states. The pure phase property guarantees that the pulse can excite spins with a constant phase across the selected region. Furthermore, the REBURP pulse has some unique behaviors, for example, self-refocusing.<sup>14,16</sup> Manipulations of spin can be described as evolution trajectory in the Bloch sphere, trajectories of spins with various frequencies are different during the exciting process. After the operation of self-refocusing pulses, trajectories of different spins, which are within the selected excitation range, can be refocused to the same destination.<sup>14,16</sup> The self refocusing behavior make REBURP pulse have almost equal excitation effects in the selected region, where all the spins can be inverted simultaneously by the pulse with high fidelity.

The spin response spectra can exhibit the main properties of REBURP pulse, and the z components of the responses spectra are depicted in Fig. 2(d). Such response can be calculated by sequentially calculating the quantum transformation within each time slice in the rotating frame. The flat bottom of the spin response spectra is the selected excitation region, and the almost equal responses indicate the self-refocusing behavior of the REBURP pulse. The band-selective property is revealed by the sharp transition edges, which bridges the flat bottom and the suppression region. Spins outside the transition edges, can keep nearly unaffected after the operation, as the unwanted excitations are well suppressed. The excellent properties of REBURP pulse make it have large applicability in practice, such as spin-echo experiments, multidimensional spectroscopy, and magnetic resonance imaging, as well as quantum gates.<sup>36</sup>

We implement experiments with REBURP shaped pulse to verify its spin response characters and test its controlling effects. Since just the amplitude of the microwave is modulated in REBURP pulse, only one set of microwave source and path is required. The shaped pulse, as well as rectangular pulses, is acquired by modulating the carrier frequency MW using an arbitrary waveform generator (Tektronix AWG430) through mixers.

The spin response characters are studied by frequency-sweeping experiment, which are similar to pulse ODMR.<sup>37</sup> After initialing to  $m_s = 0$  state by laser pulse, the NV electron spin is excited by a  $\pi$  pulse, which is rectangular pulse (in Pulse ODMR) or REBURP pulse (in our experiment). The microwave frequency is swept across the  $^{14}\text{N}$  hyperfine spectra shown in Fig. 1(b), and the electron spin state is read out after excitations.

We choose a 800 ns duration pulse, of which the flat bottom in spin response spectra (Fig. 2(d)) can just cover all the 3 dips in the spectra. By simulating the frequency-sweeping process, we can see that the three transitions are driven one

by one in Fig. 3(a). A stepwise drop and a subsequent stepwise rise emerge in the response profile, and the experiment results are shown in Fig. 3(b) in comparison with simulation. We can also get different band-width pulses by changing the pulse durations, with their simulation and experimental results of the frequency-sweeping experiment shown in Figs. 3(c) and 3(d).

In the results of frequency-weeping, steps of the profiles indicate that one or two of the transitions can be completely flipped without disturbing others, owing to the sharp edges in the spin response spectra of the REBURP pulse (Fig. 2(d)). This phenomenon confirms the band-selective property of the REBURP pulse. The central dip with triple step depths indicates that the three transitions can be perfectly excited simultaneously. This is owing to the self-focusing behavior, which induces a wide and flat bottom in the spin response spectra. The main properties of the REBURP pulse are confirmed by the consistence between experiment and simulation.

To further test the improvement of control fidelity brought by the shaped pulse, multi-flip experiment is employed under a specified circumstance with six contiguous dips in ODMR spectra (Fig. 1(c)), which is to simulate 6.5 MHz level spilling induced by an adjacent  $^{13}\text{C}$  nuclear spin. Because the NV center investigated is a pure center without ambient  $^{13}\text{C}$ , this spectrum is achieved by adjusting the external permanent magnet. The target of this experiment is to flip the three levels in the left side of the spectra, while the ones in the right side remain intact. The spin states after increasing number of flips are all read out by sequence scheme depicted in Fig. 4(a).

Several Rabi oscillations driven by rectangular pulses are implemented to determine rectangular  $\pi$  pulses, one of them shown in Fig. 4(b). Obviously, there are serious beatings caused by off-excitations with different detunings. The wide sinc-like spin response spectrum (Fig. 2(b)) of the rectangular pulses makes it impossible to drive the three energy levels in the left side synchronously without disturbing the three ones in the right side. Multi-flip tests using rectangular  $\pi$  pulses with different durations are carried out, but the

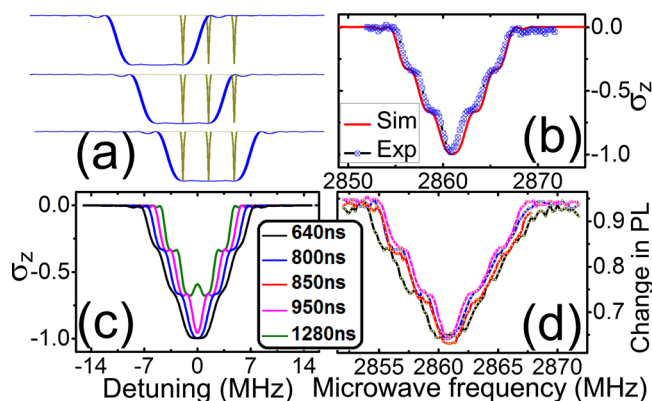


FIG. 3. Spin response of the frequency-sweeping experiment. (a) Frequency-sweeping process across  $^{14}\text{N}$  hyperfine spectra (with 3 dips) driven by the REBURP pulses. (b) Comparison of the simulation and experimental results about a 800 ns duration pulse. (c) Simulation results and (d) experimental results of different duration (640 ns, 800 ns, 850 ns, 950 ns, and 1280 ns) pulses.

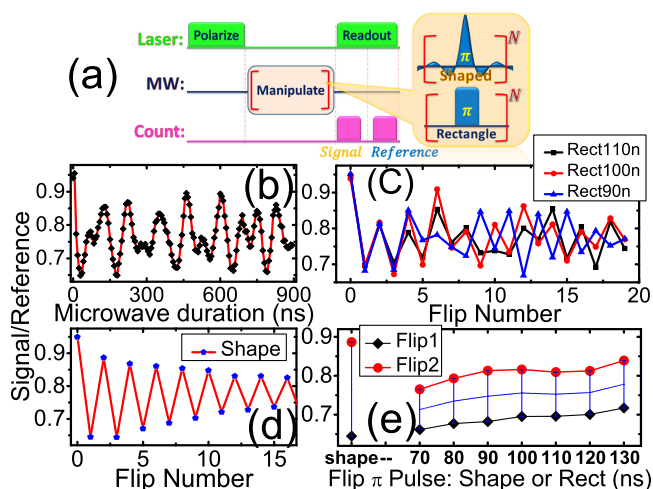


FIG. 4. Multi-flip effects of rectangular and shaped pulse. (a) The sequence scheme of multi-flip experiment. (b) Serious beating in Rabi oscillation driven by rectangular pulses. (c) Multi-flip operated by rectangular  $\pi$  pulses of different durations. (d) Multi-flip operated by REBURP shaped pulses. (e) Comparison of Flip1 and Flip2 between the shaped pulse and rectangular pulses of different durations.

curves become totally a mess after only a few flips. The best three ones are selected, as shown in Fig. 4(c). Meanwhile, multi-flip by REBURP shaped pulse is also implemented, for comparison, and it can flip at least 16 times in Fig. 4(d), indicating a far better fidelity than rectangular pulses.

We choose the second flip to evaluate the efficiency of multi-flip. Because the final state after one flip (Flip1) is just the initial state of the second flip, the respective amplitude of second flip is the difference between state after Flip1 and two flips (Flip2). The respective flip amplitude during Flip1 and Flip2 are compared among the shaped pulse and rectangular  $\pi$  pulses of different durations, as shown in Fig. 4(e). Obviously, the flip amplitudes of all the rectangular  $\pi$  pulses with different durations are much lower than (about half of) that of the shaped pulse. Based on its superiorities in flip numbers and amplitudes, we can conclude that the control fidelity is improved more than twice by the shaped pulse, compared with the traditional rectangular pulses.

The ODMR spectra with six contiguous dips employed in multi-flip experiment is just the circumstance which is used in Ref. 36. In that paper, a dominant source of errors originates from the imperfect controlling pulses. According to our experiments, the control fidelity can be improved to more than twice by the REBURP shaped pulse. Furthermore, due to its uniform response, REBURP pulse can be used to manipulate unknown initial states. Pure-phase properties of the REBURP pulse can further reduce phase errors during the manipulation. Just modulating amplitude of the microwave, one set of microwave source and path is adequate for experiments. These features make the application of REBURP pulse more robust and easy access. REBURP pulse is a good choice to implement quantum gates, as well as other applications, which require high fidelity  $\pi$  pulse such as quantum sensing by dynamic decoupling.

In summary, we have introduced a technique, REBURP shaped pulse, to improve the control fidelity, which is verified by experiments as well as simulation, in the NV spin system. The REBURP pulse has many excellent properties,

such as self-focusing, band-selective, uniform response, and pure-phase. It has almost equal excitation effect in a wide-band excitation region with sharp transition edges, while unwanted off-resonant excitations beyond the region are well suppressed. These spin response characters are confirmed by frequency-sweeping experiments. In multi-flip experiments, the repeatedly flip numbers and amplitudes of the REBURP shaped pulse both have great advantages over traditional rectangular pulses. The control fidelity is greatly improved by the shaped pulse. Furthermore, besides NV system in diamond, this universal approach can also be used for various applications such as quantum metrology, quantum sensing, and quantum information process.

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