Unambiguous nuclear spin detection using engineered quantum sensing sequence

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Sensing, localising and identifying individual nuclear spins or frequency components of a signal in the presence of a noisy environments requires the development of robust and selective methods of dynamical decoupling. An important challenge that remains to be addressed in this context are spurious higher order resonances in current dynamical decoupling sequences as they can lead to the misidentification of nuclei or of different frequency components of external signals. Here we overcome this challenge with engineered quantum sensing sequences that achieve both, enhanced robustness and the simultaneous suppression of higher order harmonic resonances. We demonstrate experimentally the principle using a single nitrogen-vacancy center spin sensor which we apply to the unambiguous detection of external protons.

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Introduction.— The detection of single nuclear spins represents an important yet challenging step towards single molecule magnetic resonance spectroscopy and imaging [1] which holds the promise for the observation of individual protein structures without the need for crystallization of large ensembles. The achievement of this goal may have significant impact on structural biology and medical imaging and may also provide a new tool for the investigation of nuclear spin dynamics in non-trivial quantum biological processes [2, 3]. Recently, research has made impressive progress in single nuclear spin detection using various physical platforms [4–8], particularly in the highly challenging task of detecting single spins in external molecules [9–14]. Among those physical platforms, a sensor based on individual negatively charged nitrogen-vacancy (NV) centers in diamond [15, 16] has demonstrated appealing prospects for applications in biology and medicine, due to its biocompatibility, nano-scale size and long coherence times under ambient conditions [17, 18]. NV centers, shallowly implanted to within a few nanometers below the diamond surface, enable strong coupling between NV sensors and target nuclei, thereby promoting the detection sensitivity from a relative large ensemble of nuclei [9, 10] to single nuclear spin sensitivity in small clusters of nuclear spins [11–14]. Besides the interest in single molecule magnetic resonance spectroscopy and imaging, single nuclear spin addressing also has an important role to play in the precise coherent control of nuclear spin qubits, where it may facilitate the realisation of quantum memories with long coherence times and nuclear spin based quantum information processors [19–22].

One ultimate goal of single molecule magnetic resonance spectroscopy using a single spin sensor is to detect a single nuclear spin and further infer the structure of a single molecule [23]. This would generally require a larger number of dynamical sensing pulses [24] such that even tiny pulse errors may accumulate and deteriorate significantly the magnetic resonance spectroscopy signal [25–30]. Furthermore, the effect of a finite pulse duration, during which the control pulses and the interaction with the nuclei/field simultaneously act on the sensor, leads to spurious higher order resonances in the measurement data that may lead to a misidentification of frequency components in the signal. Indeed, as a prominent recent example these spurious resonances have recently been identified as the source for the misidentification of nuclei in work towards nuclear magnetic resonance spectroscopy of biological systems [34]. In particular, the ratio of gyromagnetic moments μH/μC ≃ 4 of hydrogen (1H) and carbon (13C) which leads to the overlap of different resonances preventing their unique attribution to specific nuclei [34]. The presence of 13C as part of the target molecule or the diamond itself is difficult to avoid making this an urgent problem to address [36].

In this work, we both theoretically and experimentally demonstrate quantum sensing pulse sequences with engineered phases that effectively suppress spurious higher order resonances and are, at the same time, robust to pulse errors. In particular, we find that a type of MLEV-8 pulse sequence [37] denoted as YY8 sequence (\( \frac{\pi}{2} \)) - \( \left([\sigma\frac{\pi}{2}][\sigma\frac{\pi}{2}][\sigma\frac{\pi}{2}][\sigma\frac{\pi}{2}][\sigma\frac{\pi}{2}][\sigma\frac{\pi}{2}][\sigma\frac{\pi}{2}][\sigma\frac{\pi}{2}]\right)^N - \left(\frac{\pi}{2}\right)\) as a representative example can eliminate unwanted higher order spurious harmonic response in nuclear magnetic resonance spectroscopy and additionally can exhibit enhanced robustness. Using single nitrogen-vacancy spin sensor in diamond, we demonstrate the simultaneous suppression of both the 2\( ^{nd} \) and the 4\( ^{th} \) order spurious resonance e.g. from the surrounding 13C nuclei in diamond in proton sensing. We also observe the effect of the initial phase \( \phi_i \) in the XY8 family pulse sequences (\( \frac{\pi}{2} \)) - \( \left([\sigma\frac{\pi}{2}][\sigma\frac{\pi}{2}][\sigma\frac{\pi}{2}][\sigma\frac{\pi}{2}][\sigma\frac{\pi}{2}][\sigma\frac{\pi}{2}][\sigma\frac{\pi}{2}][\sigma\frac{\pi}{2}]\right)^N - \left(\frac{\pi}{2}\right)\) [35]. By choosing appropriate initial phase \( \phi_i \), either the 2\( ^{nd} \) or
pulses where each bar refers to a π sequence of and ωπ results is also applicable for quantum sensing with the other two-interval, may lead to spurious high-order resonance signal.

π pulse sequence consisting of an external magnetic field, and produce a contribution to the Hamiltonian and pulsed action. In the context of nuclear the initial state (i.e. the initial phase of the π rotation around the axis cos θ, sin φ, 0) realized in the time duration [t0, t0 + τ] is achieved by choosing Ω(t) = Ω and φ(t) = φ for t ∈ [t0, t0 + τ], with τd = θ/Ω. In the case that the microwave Rabi frequency Ω is much larger than the hyperfine interaction, the corresponding evolution operator of a (π) rotation is $U_{π}^2 = \cos φπ + \sin φπ$. Under realistic conditions, due to the finite power of the microwave acting on the NV center, the π-pulses always have a finite width (as opposed to instantaneous pulses), which can lead to spurious harmonic response and thus the possible ambiguity in the identification of nuclei [34]. Such an effect becomes particularly prominent in single-molecule magnetic resonance spectroscopy as a large number of pulses is required to get a resonance signal from weakly coupled nuclei.

To overcome such a serious obstacle, we need to carefully engineer quantum sensing pulse sequence. In order to illustrate the basic idea, we first consider a classical oscillating field $H_{osc} = A_{osc} \sin(\omega_{osc} t)\hat{z}$ with a frequency $\omega_{osc} = \omega_z/2$, see Fig. 1(c). We prepare the NV spin sensor into the initial state as $|φ^+\rangle = (|0\rangle + e^{iφ} |−1\rangle) / \sqrt{2}$. As the pulse has a finite width, the corresponding evolution of the spin sensor state is not a perfect π-rotation around the $\hat{z}$ or $\hat{y}$. Instead, the real evolution can be described by a set of rotations in the form of $R_θ = \exp(-iθ_i{\hat{H}} \cdot \sigma/2)$, where $σ$ is the spin operator and $θ_i = π + i/2$ $β_k^2 + O(β_k^4)$, $R_θ = (\cos β_k \cos φ_k, \cos β_k \sin φ_k, \sin β_k)$ and $β_k ≈ A_{osc} \sin(|ω_k|/Ω) ≪ 1$, $t_k$ is the moment when the pulse is applied. Such imperfection in pulses give rise to spurious resonance signal. For the XY8 pulse sequence, in the scenario that we are interested in, namely $A_{osc}/Ω ≪ 1$, the total evolution for one cycle is $U_{2π} = \prod_{k=1}^{K} R_{θ_k} = (1 - 8β_k^2)^I + i2 \sqrt{2} β_k (σ_x - σ_y)$, where $β_k = A_{osc} / Ω$. This leads to a 2nd harmonic response signal $P_{2ω} = 8 \left| 1 - \sin(2φ) \right| β_k^2 + O(β_k^4)$ [34, 35], which spuriously indicates a frequency component that is twice of the real oscillating field frequency. Similar analysis shows that the 4th harmonic response signal is $P_{4ω} = 2(2 - \sqrt{2}) \left| 1 + \sin(2φ) \right| β_k^2 + O(β_k^4)$ [34, 35]. It can be seen that by changing the initial phase φ, 2nd and 4th harmonics can be suppressed respectively, as $P_{2ω}$ vanishes when $φ = π/4$ while $P_{4ω}$ goes to zero when $φ = 3π/4$. This may require extra experiment complexity.

We find that a type of MLEV-8 pulse sequence $\left[ (π)_{−y} (π)_{+x} (π)_{−y} (π)_{+x} (π)_{−y} (π)_{+x} (π)_{−y} (π)_{+x} \right]^3$ (for simplicity we call it as YY8 pulse sequence) can suppress both 2nd and 4th harmonic signals simultaneously and thus reduce the experiment complexity. Using YY8 pulse sequence, the cycle evol.
The probability that the NV spin remains in the initial state \( P_0 = 1 - P(N\tau) \) is the signal observed in our NV-based nuclear magnetic resonance experiments, which provides us information on the nuclear spin, such as the type of nuclei and the hyperfine interaction with the NV spin sensor.

In our experiment, we polarize and read out the NV center spin in type IIa diamond (with natural abundance of \(^{13}\text{C}\)) using optical techniques. The microwave control pulses are generated using an arbitrary wave generator (Tektronix AWG70002A) and is amplified by an 80W microwave amplifier using a same channel. This allows us to avoid the amplitude imbalance between pulses, which otherwise would affect the robustness of YY8 pulse sequence [39]. Therefore, YY8 pulses may be more robust than XY8 sequence as is also evidenced by our numerical simulation [38]. The amplitude and phase are tuned to implement the engineered quantum sensing pulse sequences. We apply a magnetic field (510G) along the NV axis, under which condition the associated \(^{14}\text{N}\) can be polarized to improve the sensing signal, and use \(|m_f = 0\rangle\) and \(|m_i = -1\rangle\) as quantum probe in our sensing experiments. We first measure the magnetic resonance signal of \(^{13}\text{C}\) nuclear spin using XY8 and YY8 pulse sequences, see Fig.2. It can be seen that the signal is almost independent on the initial phase, and both XY8 and YY8 pulse sequences demonstrate similar

\[
H_0 = DS_z^2 - \gamma_e B_z S_z, \tag{3}
\]

where the zero-field splitting is \(D/2\pi = 2.87\text{GHz} \), \(\gamma_e\) is the electron gyromagnetic ratio, \(S\) is the spin-1 operator. As an example, we consider the detection of \(^{13}\text{C}\) nucleus in bulk diamond. The hyperfine interaction between the NV center spin and the nuclear spin is described by

\[
H_1 = S_z \sum_j A_j \cdot \hat{I}_j = S_z \sum_j (a_j \hat{I}_z^j + a_j^* \hat{I}_z^j), \tag{4}
\]

where \(a_j^*\) and \(a_j\) are the longitudinal and transversal components of the hyperfine interaction. The hyperfine interaction will cause an effective fluctuating magnetic field with a characteristic frequency that is equal to the Larmor frequency of the nuclear spin. The transition probability of the NV spin state at time \(T\) is thus given by \(P(T) = \langle \phi\mid T_{\phi} \sum \langle\psi\mid U(\phi^*) \langle\phi^* | \rho_N | U^\dagger \rangle | \phi^* \rangle\), where \(U\) is the evolution operator, \(\rho_N\) represents the initial state of the nuclear spins. The probability that the NV spin remains in the initial state

\[
P_{2\phi} = 4 [1 - \cos(2\phi)] \beta_0^2 + O(\beta_0^4)
\]

\[
P_{4\phi} = (2 - \sqrt{2}) [1 - \cos(2\phi)] \beta_0^2 + O(\beta_0^4)
\]

It can be seen that the 2
\(\phi\) and 4
\(\phi\) harmonic signal can thus be simultaneously suppressed up to second-order when the initial phase is chosen as \(\phi = 0\) [38]. We remark that YY8 pulse sequence can suppress the other spurious resonances, including the (4/5)\(\phi\), (2/3)\(\phi\) and (4/3)\(\phi\) response, in contrast with XY8 pulse sequence [38].

Unambiguous nuclear spin detection.— Using an NV center spin sensor in diamond, we demonstrate experimentally the suppression of spurious high-order response signals in the detection of nuclear spins using engineered quantum sensing pulse sequences. The NV center is a point defect in diamond, which has a triplet ground state manifold with the spin quantum number \(m_s = 0, \pm 1\). In NV-based nuclear magnetic resonance experiments, one applies a magnetic field \(B_z\) along the NV axis that connects the nitrogen atom and the vacancy site, the NV center spin Hamiltonian is given as follows [15]

\[
H_0 = DS_z^2 - \gamma_e B_z S_z, \tag{3}
\]

where the zero-field splitting is \(D/2\pi = 2.87\text{GHz}\). \(\gamma_e\) is the electron gyromagnetic ratio, \(S\) is the spin-1 operator. As an example, we consider the detection of \(^{13}\text{C}\) nucleus in bulk diamond. The hyperfine interaction between the NV center spin and the nuclear spin is described by

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H_1 = S_z \sum_j A_j \cdot \hat{I}_j = S_z \sum_j (a_j \hat{I}_z^j + a_j^* \hat{I}_z^j), \tag{4}
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where \(a_j^*\) and \(a_j\) are the longitudinal and transversal components of the hyperfine interaction. The hyperfine interaction will cause an effective fluctuating magnetic field with a characteristic frequency that is equal to the Larmor frequency of the nuclear spin. The transition probability of the NV spin state at time \(T\) is thus given by \(P(T) = \langle \phi\mid T_{\phi} \sum \langle\psi\mid U(\phi^*) \langle\phi^* | \rho_N | U^\dagger \rangle | \phi^* \rangle\), where \(U\) is the evolution operator, \(\rho_N\) represents the initial state of the nuclear spins. The probability that the NV spin remains in the initial state

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P_{2\phi} = 4 [1 - \cos(2\phi)] \beta_0^2 + O(\beta_0^4)
\]

\[
P_{4\phi} = (2 - \sqrt{2}) [1 - \cos(2\phi)] \beta_0^2 + O(\beta_0^4)
\]
using YY8 pulse sequence. (FIG. 4. (Color online) Detection of $^1$H magnetic resonance signal using YY8 pulse sequence. (a) The spectrum as measured by a shallow NV center spin for various magnetic field. (b) The frequency of peak response as a function of the magnetic field $B$. The red line has a slope $4.20\pm0.13$ kHz/G that gives an estimated gyromagnetic ratio of $^1$H. The Rabi frequency is $\Omega = (2\pi)25$ MHz.

We further test the suppression of spurious high-order resonance signals using engineered pulse sequences. In Fig.3, we plot the dependence of the 2nd and 4th harmonic signals on the initial phase $\phi$ using the YY8 pulse (d-f) sequence as compared with the XY8 sequence (a-c). It can be seen that the spurious high-order resonance signals can be suppressed by choosing approximate initial phases of XY8 and YY8 pulse sequences, in which YY8 pulse sequence demonstrates better performance over XY8 pulse sequence. By choosing $\phi = 0$, both 2nd and 4th harmonics are suppressed simultaneously using YY8 pulse sequence, see Fig.3(d-f), while this cannot be achieved for any choice of $\phi$ for the XY8 sequence, see Fig.3(a-c). The amplitude of spurious high-order resonance signals are also relatively smaller using YY8 pulse sequence even when the initial phase is not perfect. These advantageous features of YY8 pulse sequence allows for the efficient unambiguous identification of nuclear spins, in particular it implies that YY8 pulse sequence can unambiguously identify the signal from $^1$H, while avoiding the possible confusion with the 4th harmonic signal of $^{13}$C with no extra experiment requirement as compared with the already widely used XY8 pulse sequence.

We then use YY8 pulse sequence with the initial phase $\phi = 0$ to detect the magnetic resonance signal of $^1$H in oil on diamond surface. The shallowly implanted NV centers are created by a 2.5 keV N+ ions into type IIa diamond. The Ramsey and spin echo measurement indicates that the NV center shows $T_2^+ \approx 300$ns and $T_2 \approx 5$µs. In Fig.4(a), we measure the spectrum recorded by YY8 pulse sequence at different magnetic fields. The scaling of the peak frequency with the magnetic field is shown in Fig.4(b). The linear slope of the frequency $4.20 \pm 0.13$ kHz/G fits well with the gyromagnetic ratio of $^1$H ($4.258$ kHz/G). As we show above, the YY8 pulse sequence can effectively suppress the high-order spurious response, and therefore our measurement provides a way to detect $^1$H unambiguously. As $^1$H magnetic resonance spectroscopy is very important in various scenarios, the present engineered quantum sensing pulse sequence, particularly YY8 pulse sequence, may find useful applications in single-molecule magnetic resonance spectroscopy using quantum spin sensor.

Conclusions— We implement engineered quantum sensing pulse sequences that suppress spurious higher order resonances, a feature that will find application in unambiguous nuclear spin detection and more generally the identification of frequency components of externally applied signals. Specifically, this eliminates the ambiguity in the nuclear magnetic resonance signal of single nuclear spin detection that is inherent to pulsed schemes due to the duration of individual pulses. The YY8 pulse sequences shows better performance in suppressing spurious response and are even more robust against the pulse errors than the widely used XY8 pulse sequences (e.g amplitude error). The simplicity and advantageous features of this type of pulse sequences make them an appealing choice for the applications in nuclear spin detection as well as the quantum control of nuclear spin registers.

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