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ABSTRACT

We analyze the scale factor linearity, steady-state, transient, and noise characteristics of a nuclear magnetic resonance oscillator coupled with the phase-locked loop, which makes its performance improvement possible by a balanced strategy in optimizing parameters based on the proposed model. The numerical simulation indicates that the simple oscillator system gives a better scale factor linearity and transient response than the coupled system, while the steady-state solution is similar between the two with experimental validation. The phase and magnetic noise suppression is necessary to ensure the dynamic response of the coupled system. The characteristic analysis not only facilitates the rapid-response optimization of the coupled oscillator system under a dynamic environment but also enlightens corresponding steady-state tracking precision.

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I. INTRODUCTION

High performance nuclear magnetic resonance (NMR) oscillators benefit various applications such as NMR spectroscopy,1–4 magnetic resonance imaging (MRI),5–7 and the NMR gyroscope.8–11 The Larmor precession frequency of the detected nuclear species is utilized to enable the signal detection of the NMR oscillator, which is further achieved by measuring nuclear spins with the built-in magnetometer.12 The nuclear spin of a single atom is too weak to be detected by currently available methodology; thus, an ensemble of atoms is applied as the sensitive medium to be hyperpolarized by spin exchange optical pumping (SEOP)13–15 to form the detectable macroscopic magnetization vector along the longitudinal direction. Furthermore, a transverse magnetic field that matches the Larmor frequency of the detected nuclear species needs to be applied to make the magnetization vector precess around the longitudinal direction, thus enabling the Larmor frequency detection by tracking the applied transverse field.

To achieve high performance NMR oscillators, it is crucial to track the Larmor frequency precisely in time with an appropriate tracking approach, e.g., fast Fourier transform (FFT) and phase-locked loop (PLL). The PLL technique is widely used within the field of signal processing, especially applicable for real-time dynamic environment applications.16 Thus, understanding the characteristics of the coupling between the NMR oscillator and the corresponding tracking approach becomes important. Besides well-known characteristics of the typical PLL technique,16 the steady-state characteristic analysis of the NMR oscillator has also been reported. However, the characteristics of the NMR oscillator coupled with tracking approaches have not been analyzed. The characteristic analysis of the coupled system is not only crucial to optimize its dynamic response but also enlightens its tracking precision. In this paper, we perform a characteristic analysis of the coupled system compared with the pure oscillator, including scale factor linearity, steady-state, transient, and noise characteristics.

II. THEORETICAL MODEL

The phase characteristic equation of the NMR oscillator is concluded as follows:17

\[
\frac{d\phi(t)}{dt} = \Omega_2(t) - \Gamma_2 \tan[\phi(t) - \theta(t)],
\]  

(1)
where \( \phi(t) \) and \( \theta(t) \) denote the phase of its input and output signals applied to the transverse field, respectively. \( \Gamma_2 = 1/T_2 \) denotes the transverse relaxation rate of the sensitive atoms, where \( T_2 \) denotes the corresponding transverse relaxation time. \( \Omega_2(t) = \gamma B(t) \) denotes the effective Larmor precession frequency of the sensitive atoms along the longitudinal direction, where \( \gamma \) denotes the gyromagnetic ratio of the sensitive atoms and \( B(t) \) denotes the longitudinal magnetic field.

To analyze its characteristics in frequency domain with transfer function, not only should the variables be redefined as \( \Delta \phi(t) = \phi(t) - \phi(0) \), \( \Delta \Omega_2(t) = \Omega_2(t) - \Omega_2(0) \), and \( \Delta \theta(t) = \theta(t) - \theta(0) \) to satisfy the zero initial condition, but also the nonlinearity of Eq. (1) needs to be approximated into the linearized form, which is always satisfied with a low angle condition. Thus, the modified form is as follows:

\[
\frac{d \Delta \phi(t)}{dt} = \Delta \Omega_2(t) + \Gamma_2 [\Delta \theta(t) - \Delta \phi(t)], (2)
\]

from which the form in frequency domain can be obtained through the Laplace transform as

\[
s \Delta \phi(s) = \Delta \Omega_2(s) + \Gamma_2 [\Delta \theta(s) - \Delta \phi(s)], (3)
\]

which leads to the system transfer function of the NMR oscillator as

\[
H(s) = \frac{\Delta \theta(s)}{\Delta \phi(s)} = \frac{(s + \Gamma_2) \Delta \theta(s)}{\Delta \Omega_2(s) + \Gamma_2 \Delta \theta(s)}. (4)
\]

On the other hand, we focus on the mostly applied second-order PLL as the tracking approach, which typically consists of a phase detector (PD), a loop filter (LF), and a voltage-controlled oscillator (VCO), while a similar procedure can be obtained with other types of PLL or tracking approaches. The typical system transfer function of the second-order PLL is as follows:

\[
H(s) = \frac{2 \xi \omega_n s + \omega_n^2}{s^2 + 2 \xi \omega_n s + \omega_n^2}, (5)
\]

where \( \omega_n \) denotes the undamped natural frequency of the system and \( \xi \) denotes the dimensionless damping coefficient of the system. If the NMR oscillator is coupled with the second-order PLL, the corresponding transfer function structural diagram is depicted as in Fig. 1, where the phases of the input and output signals in time domain are denoted as \( \theta_i(t) \) and \( \theta_o(t) \), respectively. \( \theta_i(t) = \theta_i(t) - \theta_i(t) \) denotes the phase error, which leads to the output voltage of PD as \( \mathcal{V}_{PD}(t) = K_d \sin[\theta_i(t)] \), where \( K_d \) denotes the gain factor of PD, and the corresponding linearized form could be obtained as \( \mathcal{V}_{PD}(t) = K_d \theta_i(t) \) under the case of low phase error. \( K_1 \) and \( K_2 \) denote the proportionality and integral coefficient of the LF, respectively, which leads to the output voltage of LF as \( \mathcal{V}_{LF}(t) = (K_1 + f K_2) \mathcal{V}_{PD}(t) \). The VCO converts \( \mathcal{V}_{LF}(t) \) into the frequency output \( \Delta \omega(t) = d \theta(t)/dt = K_v \mathcal{V}_{LF}(t) \), where \( K_v \) denotes the gain factor of VCO. The variables shown in Fig. 1 are all Laplace transform of the abovementioned variables. \( \Delta \omega_o(s) = s \theta_i(s) \) and \( \Delta \omega_o(s) = s \theta_o(s) \) denote the Laplace transform of the output frequency of the NMR oscillator and the coupled system, respectively, which also satisfy the zero initial condition as \( \Delta \omega_o(t) = \omega_o(t) - \omega_o(0) \) and \( \Delta \omega_o(t) = \omega_o(t) - \omega_o(0) \). The coupled system leads to the inverse input and output for the NMR oscillator which satisfy \( \Delta \phi(s) = \theta_i(s) \) and \( \Delta \theta(s) = \theta_o(s) \), respectively. Substituting Eq. (5) into Eq. (4), the output frequency of the NMR oscillator and the coupled system with respect to the effective Larmor frequency in frequency domain are obtained, respectively, as follows:

\[
\Delta \omega_o(t) = \frac{s^2 + 2 \xi \omega_n s + \omega_n^2}{s^2 + (2 \xi \omega_n + \Gamma_2) s + \omega_n^2} \Delta \Omega_2(s), (6)
\]

\[
\Delta \omega_o(t) = \frac{2 \xi \omega_n s + \omega_n^2}{s^2 + (2 \xi \omega_n + \Gamma_2) s + \omega_n^2} \Delta \Omega_2(s). (7)
\]

### III. SCALE FACTOR LINEARITY

We perform numerical simulations according to the typical parameters listed in Table 1 with Eqs. (6) and (7) to show the scale factor amplitude-frequency response of the NMR oscillator and the coupled system, as shown in Figs. 2 and 3, respectively.

Figure 2 shows that the scale factor amplitude-frequency response of the NMR oscillator serves as a notch filter, the amplitude of which is almost 1 in most cases, and the corresponding stop band becomes broader with increasing \( \omega_n \), while its central frequency remains constant. Furthermore, the amplitude-frequency response increases and the stop band becomes broader with increasing \( \Gamma_2 \) at 11.86 Hz, whereas the central frequency remains constant.

Figure 3 shows that the scale factor amplitude-frequency response of the coupled system serves as a low-pass filter with

### Table 1: Simulation parameters. Typical values are chosen for the parameters of the PLL and the NMR oscillator.

| Parameter  | Value            |
|------------|------------------|
| \( \omega_n \) | 1.0 (rad/s)      |
| \( \xi \)   | 0.707            |
| \( \Gamma_2 \) | 0.01 (Hz)        |
| \( \gamma \) | \( 2 \pi \times 11.86 \) [rad/(s μT)] |
FIG. 2. The scale factor amplitude-frequency response of the NMR oscillator with different (a) \( \omega_n \), (b) \( \xi \), and (c) \( \Gamma_2 \). Solid lines: simulation results. Legends: the values of \( \omega_n \), \( \xi \), and \( \Gamma_2 \).

FIG. 3. The scale factor amplitude-frequency response of the coupled system with different (a) \( \omega_n \), (b) \( \xi \), and (c) \( \Gamma_2 \). Solid lines: simulation results. Legends: the values of \( \omega_n \), \( \xi \), and \( \Gamma_2 \).

an amplitude of 1, the cut-off frequency of which increases with increasing \( \omega_n \), as depicted in Fig. 3(a). On the other hand, Fig. 3(b) indicates that the medium-frequency gain decreases while the cut-off frequency remains constant with increasing \( \xi \). Furthermore, the medium-frequency gain and the cut-off frequency both decrease with increasing \( \Gamma_2 \), as shown in Fig. 3(c).

In conclusion, the NMR oscillator gives much better scale factor linearity than the coupled system in frequency domain in most cases.
Higher values of $\omega_n$ and $\xi$ and moderate $\Gamma_2$ are preferred to achieve a better scale factor linearity and broader bandwidth of the NMR oscillator and the coupled system.

**IV. OSCILLATING FREQUENCY IN EQUILIBRIUM**

Note that the coupled system would reach the steady-state with stable phase error, which leads to the equation $d(\theta_i(t) - \theta_o(t))/dt = 0$, i.e., $\Delta \omega_o(t) = \Delta \omega_i(t)$. Assuming an existing system-delay induced phase shift $\beta$, by substituting the PLL equations into Eq. (1), the output frequency of the coupled system in equilibrium can be expressed as

$$
\omega_o(t) = \omega_o(0) + \Delta \Omega_z(t) - \Gamma_2 \tan \left[ \arcsin \frac{\omega_o(t) - \omega_o(0)}{2 \xi \omega_n} - \beta \right].
$$

Comparing Eq. (8) with Eq. (1) which describes the phase characteristics of the pure NMR oscillator, a relatively ideal PLL with a high value of $\xi \omega_n$ that satisfies $\xi \omega_n \gg [\omega_o(t) - \omega_o(0)]$ will make Eq. (8) have identical solutions with Eq. (1), which indicates that the impact of a relatively ideal PLL on the output frequency of the coupled system in equilibrium is negligible. Moreover, a nonideal PLL with a moderate value of $\xi \omega_n$ that makes $\xi \omega_n \approx [\omega_o(t) - \omega_o(0)]$ will lead to the nonlinearity of $\omega_o(t)$ with $\omega_o(0)$, which is not suitable to be described with Eq. (1) any more. On the other hand, a slow PLL with a low value of $\xi \omega_n$ that satisfies $\xi \omega_n \ll [\omega_o(t) - \omega_o(0)]$ will disable the coupled system in applications of rapid response and also make Eq. (8) have no solutions, which makes Eq. (8) one of the valid boundary conditions for the applied PLL.

To prove the validity of Eq. (8), the numerical simulation and corresponding experiment with the setup depicted in Fig. 1 are performed, where the output frequency with respect to the phase shift of the coupled system is illustrated in Fig. 4. The PLL module applied in Fig. 4 was achieved with the parameters listed in Table 1 by a lock-in amplifier (Zurich Instruments HF2LI 1070), while the NMR oscillator was home-built with the setup shown in Fig. 5.

In Fig. 5(a), two distributed feedback lasers (UniQuanta DFB801-D) were orthogonally placed that emitted linearly polarized laser beams at 794 nm. One of the lasers (pumping laser) was utilized to emit the pump beam, with circular polarization by a quarter-wave plate; meanwhile, the other (probe laser) was utilized to emit the probe beam, with the polarization being rotated by a half-wave plate. A vapor cell filled with condensed rubidium atoms ($^{87}$Rb), and buffer gases consisting of 10 Torr Xe in natural isotopic abundance and 300 Torr N$_2$ as a quencher, was placed in the center. Passing through the vapor cell, the probe beam was separated by a polarization beam splitter (PBS) into two mutually perpendicular linearly polarized beams. To extract the detected signal from the NMR oscillator, the Faraday rotation angle of the probe beam was obtained by two photodiodes (PDs) (Hamamatsu, S6775) forming the configuration of the balanced photodetector (BPD).

Three mutually perpendicular magnetic coils were used in producing magnetic fields. A high performance magnetic shield,
originally made of high permeability material (Mumetal), was built outside the magnetic coils in mitigating the impact of the stray magnetic field and its fluctuations. Moreover, an oven with Kapton heating film was applied as the heater to vaporize atoms in the vapor cell.

Figure 5(b) gives a brief phenomenological physical diagram of the NMR oscillator. The pump light and static magnetic field $B_0$ along the Z-axis polarized the sensitive atoms to form the macroscopic magnetization vector, while the transverse alternating magnetic field $B_x$ along the X-axis made the magnetization vector precess along the Z-axis to enable the Rb-Xe comagnetometer as the NMR oscillator.

Figure 4 shows that the numerical simulation matches the experimental result well, which proves that Eq. (8) can predict the steady-state output frequency of the NMR oscillator coupled with the PLL. Note from Eq. (8) that $\Gamma_2$ can be extracted from the matched simulation curve, which is $\Gamma_2 = 0.0072$ (Hz) in Fig. 4, giving a simple approach of measuring the transverse relaxation rate of the sensitive atoms.

V. TRANSIENT CHARACTERISTICS

On the other hand, the transient characteristics of the NMR oscillator coupled with the PLL are crucial for its application under a dynamic environment. Assuming the typical step function as the external excitation with $\Delta \Omega(t)$, which has the step amplitude $\Delta \Omega$ and corresponding Laplace transform $\Delta \Omega/s$. Thus, the output frequency of the NMR oscillator in frequency domain can be modified from Eq. (6) as

$$\Delta \omega(s) = \frac{1}{s} - \frac{\Gamma_2}{s^2 + (2\xi \omega_n + \Gamma_2)s + \omega_n^2} \Delta \Omega,$$

from which the corresponding expression in time domain could be obtained through the inverse Laplace transform as

$$\Delta \omega(t) = \Delta \Omega(1 - A_1e^{s_1t} - A_2e^{s_2t}),$$

where $A_1$, $A_2$, $s_1$, and $s_2$ can be obtained from Eq. (9). Note that the output frequency of the NMR oscillator would reach its steady-state value $\Delta \Omega$ after damped oscillation as long as $\omega_n \neq 0$. A similar expression can be obtained for the output frequency of the coupled system as follows:

$$\Delta \omega_o(t) = \Delta \Omega(1 - B_1e^{s_1t} - B_2e^{s_2t}),$$

where $B_1$ and $B_2$ can be similarly obtained as $A_1$ and $A_2$. The corresponding numerical simulations with the step excitation amplitude $\Delta \Omega = 0.05$ (Hz) given at $t \geq 5$ (s) are presented for the output frequency of the NMR oscillator and the coupled system, as depicted in Figs. 6 and 7, respectively.

Figure 6 shows that the rise time of the NMR oscillator keeps almost zero in various cases, while the stabilized time required to reach its steady-state value and the corresponding overshoot decrease with increasing $\omega_n$, as depicted in Fig. 6(a). On the other hand, Fig. 6(b) indicates that the oscillation and corresponding overshoot decrease with increasing $\xi$, whereas the stabilized time remains almost constant. Furthermore, the stabilized time and the corresponding overshoot increase with increasing $\Gamma_2$, as shown in Fig. 6(c).

Figure 7 shows that the rise time and stabilized time of the coupled system are longer than those of the NMR oscillator in various cases, where the stabilized time, rise time, and corresponding overshoot decrease with increasing $\omega_n$, as depicted in Fig. 7(a). On the other hand, Fig. 7(b) indicates that the oscillation and corresponding overshoot decrease with increasing $\xi$,
constant. As shown in Fig. 7(c), whereas the stabilized time remains almost constant. Furthermore, the rise time increases while overshoot decreases with increasing $\Gamma$ whereas the stabilized time remains almost constant. Furthermore, the rise time increases while overshoot decreases with increasing $\Gamma$ as shown in Fig. 7(c), whereas the stabilized time remains almost constant.

VI. NOISE CHARACTERISTICS

According to Eq. (8), the output frequency noise of the coupled system could arise from two typical sources, the phase noise and magnetic field noise. The total phase noise could be assumed as $\delta \theta(t) = \delta \theta_i(t) - \delta \theta_o(t)$, where $\delta \theta_i(t)$ and $\delta \theta_o(t)$ are the input and the output phase noise, respectively. Taking simply the phase noise into consideration, the relationship in frequency domain between the output frequency noise of the NMR oscillator $\delta \omega_o(s)$ and the total phase noise $\delta \theta_i(s)$ can be expressed as

$$\delta \omega_o(s) = -\Gamma \delta \theta_i(s),$$

from which the transfer function between the output frequency noise of the coupled system $\delta \omega_o(s)$ and the total phase noise $\delta \theta_i(s)$ is, by substituting Eq. (5) into Eq. (12), as follows:

$$\delta \omega_o(s) = \frac{-\Gamma (2\xi \omega_o s + \omega_o^2)}{s^2 + 2\xi \omega_o s + \omega_o^2} \delta \theta_i(s).$$

Thus, the output frequency noise characteristic of the NMR oscillator is proportional to the phase noise by a factor of $\Gamma$ according to Eq. (12), while Eq. (13) indicates a similar phase noise transfer characteristic as the PLL for the coupled system, where the latter is simulated as shown in Fig. 8.

Figure 8 shows that the frequency-phase transfer amplitude-frequency response of the coupled system serves as a high-pass filter, the cut-off frequency, and the high-frequency gain which increase with increasing $\omega_n$, as depicted in Fig. 8(a). On the other hand, Fig. 8(b) indicates that the high-frequency gain increases while the cut-off frequency decreases with increasing $\xi$. Furthermore, the high-frequency gain increases with increasing $\Gamma$, as shown in Fig. 8(c), whereas the cut-off frequency remains constant. Thus, lower values of $\omega_n$, $\xi$, and $\Gamma$ are preferred to suppress the phase noise transferred frequency noise of the coupled system.

On the other hand, the noise in the effective Larmor frequency $\delta \Omega(t) = \gamma \delta \vec{B}_o(t)$ arises from the longitudinal magnetic field noise $\delta \vec{B}_z(t)$. By substituting its Laplace transform into Eqs. (6) and (7), the expression of $\delta \omega_o(s)$ and $\delta \omega_i(s)$ with respect to $\delta \vec{B}_z(s)$ are obtained, respectively, as

$$\delta \omega_o(s) = \gamma \frac{s^2 + 2\xi \omega_o s + \omega_o^2}{s^2 + 2\xi \omega_o s + \omega_o^2} \delta \vec{B}_z(s),$$

$$\delta \omega_i(s) = \gamma \frac{2\xi \omega_o s + \omega_o^2}{s^2 + 2\xi \omega_o s + \omega_o^2} \delta \vec{B}_z(s),$$

which give the same transfer characteristics as the corresponding amplitude-frequency characteristics according to Eqs. (6) and (7) multiplied by $\gamma$, with the simulation results illustrated in Figs. 9 and 10, respectively.

In conclusion, the NMR oscillator gives better dynamic response than the coupled system under the case of same parameters. Higher values of $\omega_n$ and $\xi$ and moderate $\Gamma$ are preferred to optimize the stabilized time and corresponding rise time, oscillation characteristics, and overshoot of the coupled system to approach those of the NMR oscillator, respectively.
FIG. 8. The frequency-phase transferred amplitude-frequency response of the coupled system with different (a) $\omega_n$, (b) $\xi$, and (c) $\Gamma_2$. Solid lines: simulation results. Legends: the values of $\omega_n$, $\xi$, and $\Gamma_2$.

FIG. 9. The frequency-magnetic transferred amplitude-frequency response of the NMR oscillator with different (a) $\omega_n$, (b) $\xi$, and (c) $\Gamma_2$. Solid lines: simulation results. Legends: the values of $\omega_n$, $\xi$, and $\Gamma_2$.

an opposite strategy should be applied with preferred lower values of $\omega_n$ and $\xi$ and higher $\Gamma_2$. Figure 10 leads to similar conclusions that lower $\omega_n$ and higher values of $\xi$ and $\Gamma_2$ are preferred to suppress the magnetic noise of the coupled system.

In conclusion, lower values of $\omega_n$ and $\xi$ are both preferred to suppress the phase and magnetic noise transferred frequency noise of the coupled system, while a moderate $\Gamma_2$ should be considered to give a balanced impact between the two. On the other hand, the...
VII. CONCLUSIONS

We analyze the characteristics of a NMR oscillator coupled with the PLL to study the scale factor linearity, steady-state, transient, and noise response of the output frequency compared with the pure NMR oscillator. Numerical simulation, being experimentally validated, indicates that the NMR oscillator gives a better scale factor linearity and transient response than the coupled system under the case of same parameters, and the difference between the two could be lower with higher values of $\omega_n$ and $\xi$ and moderate $\Gamma_2$. The steady-state response of the coupled system is similar to that of the NMR oscillator, which varies with the system-delay induced phase shift and the parameters of the PLL. The phase and magnetic noise suppression is necessary to ensure the transient response of the coupled system, which requires higher values of $\omega_n$ and $\xi$. Such a demonstration makes the performance improvement possible for the NMR oscillator coupled with the PLL using a balanced strategy in optimizing the PLL parameters to relatively high values and the transverse relaxation rate of the sensitive atoms to a relatively low value, especially enabling the rapid response optimization of the coupled system under a dynamic environment. Although a better ideal NMR oscillator mode is not yet achievable, it can be treated as the ultimate limit of the coupled system mode and might be, in future works, achieved by addressing the challenge of extracting the NMR oscillator output without other tracking approaches.

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