Simulating Decoherence of a Nitrogen – Vacancy Centre Spin Qubit via Ornstein – Uhlenbeck Process

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Abstract. Owing to its remarkable optical properties and its ability to be controlled by microwave fields at room temperature, nitrogen-vacancy (NV) centre in diamond has been a promising platform for various nanotechnological applications, e.g. quantum sensing and magnetic resonance spectroscopy. The qubit associated with the NV centre ground state spin has been the key element for the realisation of such applications. Its coherence time determines the application performances, e.g. the sensitivity of the NV-qubit based quantum sensor. Due to unwanted and unavoidable interactions with noisy environment, the qubit undergoes decoherence that shortens its coherence time and hence reduces its application performance. Therefore, the investigation and mitigation of the decoherence of the NV qubit are of the utmost importance. Here, we simulate the qubit decoherence using Ornstein-Uhlenbeck process that is essential for designing a set of modulating control pulses to mitigate the effect.

1. Introduction

Quantum-based technologies develop using one of physics principles, namely quantum mechanics. One among such technologies is spectroscopy. Spectroscopy is used to observe the microscopic structure of materials and take a measurement of the materials. Of many kinds of spectroscopy, magnetic resonance is one of the spectroscopy technologies that is frequently used. In principle, magnetic resonance uses a magnetic field to detect a transition in the electronic structure of materials. There are two kinds of magnetic resonance, electron spin resonance (ESR) and nuclear magnetic resonance (NMR). The difference between them is the ESR works in the microwave regime, while the NMR is in the radio-frequency regime. The ESR/NMR uses an external magnetic field to detect electron/nuclear dynamics in the materials [1, 2].

A system of nitrogen-vacancy (NV) in diamond is a promising system for the realisations of room temperature ESR and NMR at the nanometer scale [3]. The NV centre system is an optically active color centre in diamond in which a nitrogen atom as a foreign atom or an impurity replaces the diamond's constituent carbon atom, while such a replacement induces a carbon vacancy around the Nitrogen site, both together forming a defect centre with a c_{3v} symmetry [4]. Analysis on the electronic structure of the NV centre shows that the centre's electronic ground state has a spin $S = 1$ property [5], which can be modelled by the following Hamiltonian :

$$\mathcal{H} = \hbar D\left[\hat{S}_Z^2 - \frac{2}{3}\right] + \hbar E\left(\hat{S}_X^2 - \hat{S}_Y^2\right) + \hbar\gamma_{nv}\vec{B}\cdot\hat{\vec{S}} + \hbar\delta_{\parallel}\mathcal{E}_Z\left[\hat{S}_Z^2 - \frac{2}{3}\right] - \hbar\delta_{\perp}\left[\mathcal{E}_X\left(\hat{S}_X\hat{S}_Y + \hat{S}_Y\hat{S}_X\right) + \mathcal{E}_Y\left(\hat{S}_X^2 - \hat{S}_Y^2\right)\right] + \hbar\sum_{i=1}^{n}\left(\hat{\vec{S}}\mathcal{N}_i\hat{\vec{I}}_i + \gamma_i\vec{B}\cdot\hat{\vec{I}}_i + Q_i\hat{I}_{Z,i}^2\right) \quad (1)$$

The first and second terms are called as zero field splitting (ZFS) term of Hamiltonian, which describes the NV centre state in the absence of applied magnetic field. These terms explain that there is a crystal field that happens in this system, with D is an axial zero-field parameter and E is a non-axial zero-field parameter. The third term, usually called the magnetic interaction term, explains a magnetic field interaction between the electron spin and external magnetic field with a value of $\gamma_{nv} = 2\pi \times 28\, MHz/mT$, and $\vec{B}$ is an external magnetic field [5]. There are fourth and fifth terms of the Hamiltonian, namely the electric interaction terms, describing the interaction between the electric field and spins. These terms indicate that there is an external electric field contribution equal to the effect of the crystal field on the NV centre. The sixth term, a hyperfine interaction term, is the interaction between spins in NV centre and another spin found in the NV centre, including a nuclear spin. The dominant interactions that occur are the interaction between the nucleus of the ^{15}N or ^{14}N and the nuclear spin of the ^{13}C atom. The seventh term is the nuclear Zeeman interaction term, while the last term is the nuclear quadrupole interaction.

The NV centre system is often used as a quantum–based technology platform because it can operate at room temperature. The electronic ground state can also be chosen as a two-level system forming a system of spin S = 1/2, which can be used as a quantum bit (qubit), a key ingredient for quantum information processing [6, 7]. Although, the actual state of the electronic structure of the NV centre system is the spin system S = 1, our work use only the two levels, $m_s = 0$ and $m_s = -1$. This can be done by applying a magnetic field to separate the states with $m_s = +1$ and $m_s = -1$ such that only states $m_s = 0$ and $m_s = -1$ are accessible by our process.

The physical properties of the NV centre can be determined with a measurement. The measurement use magnetic resonance technology. The basic concept of the NV centre is the ESR, which take effect during the electron spin transition. Moreover, the system can also be applied by magnetic resonance imaging (MRI) to observe the movement of spin. Also, one can observe the decoherence process caused by an applied external magnetic field. The decoherence occurs due to errors and noises during measurement and interaction. Decoherence exist when we use ESR/NMR techniques for measurement. The decoherence is a process of losing the quantum coherence, a superposition state affected by an interaction between system and environment during the time evolution. This can be classified as noise in measurement with magnetic resonance technology, where at magnetic resonance this process is known as spin-relaxation time [2, 8]. Regarding the refocusing process from spin magnetisation, there is a method to prolong the quantum coherence, namely a dynamical decoupling method [9]. The method allows one to observe the dynamics of nuclear spin rotations.

2. Model and Method

In most measurements of such a quantum system, there is always some disturbance called noise. Therefore, for theoretical modelling of the system, the calculation must involve the noise factor. For modeling the noise factor, we use a method named as Ornstein – Uhlenbeck process (O - U process). We will use this modelling method by its Hamiltonian equation, and the dynamical equation will then be solved numerically via the Lindblad master equation, or a master equation for simplicity. To perform the numerical simulations we use the Quantum Toolbox in Python (QuTiP) package [10]. The master equation is numerically simulated using Runge-Kutta solver for the partial differential equation (PDE) in QuTiP.

2.1. Ornstein – Uhlenbeck Process

For modelling the noise factor from a measurement, we use OU process. Included in the model Hamiltonian of the electronic spin state of the NV centre with $S = 1/2$.

$$\mathcal{H}_L(t) = \frac{\omega_0 + \delta(t)}{2}\sigma_z + \Omega_1 f(t)\big(1 + \epsilon(t)\big)\cos\big(\omega_0 t + \phi(t)\big)\sigma_x + \frac{g}{2}\sigma_z \cos(\omega_s t + \xi) \qquad (2)$$

With ω_0 is a Bohr transition frequency, Ω is the electron Rabi frequency, $f(t)$ is the control modulation function. The noises, $\delta(t)$ and $\epsilon(t)$ are the off-resonance error and on-resonance error respectively. ϕ denotes the phase angle of the applied field, while ξ is an unknown phase. In the presence of an external signal, $g/2$ is the signal amplitude and ω_s is the signal angular frequency [11]. To simplify the dynamics, by using interaction basis $\mathcal{H}_0^{(1)} = \omega_0\sigma_z/2$ and the Rotating Wave Approximation (RWA) with $\Omega_1 \ll \omega_0$, we arrive at the effective Hamiltonian [11],

$$\mathcal{H}(t) = \frac{\delta(t)}{2}\sigma_z + \frac{\Omega_1}{2}f(t)\big(1+\epsilon(t)\big)\big(\cos\big(\phi(t)\big)\sigma_x + \sin\big(\phi(t)\big)\sigma_y\big) + \frac{g}{2}\sigma_z\cos(\omega_s t + \xi) \tag{3}$$

The error factor, off – resonance error and on – resonance error, is stochastic function modelled by the OU process [11], as

$$\delta(t+\Delta t) = \delta(t)e^{-\frac{\Delta t}{\tilde{\tau}}} + \widetilde{n_\delta}\sqrt{\sigma_\delta^2\left(1-e^{-\frac{2\Delta t}{\tilde{\tau}}}\right)} \tag{4}$$

with $\widetilde{\boldsymbol{n_\delta}}$ is a Gaussian random number. The relation between σ_δ and T_2^* (combined time constant) is given by $\sigma_\delta = \sqrt{2}/T_2^*$, where $T_2^* = 3\mu s$ and $\tilde{\tau} = 25\mu s$ is a diffusion time constant. The on-resonance error (with $\sigma_\epsilon = 0.005$), is modelled by the OU process as

$$\epsilon(t+\Delta t) = \epsilon(t)e^{-\frac{\Delta t}{\tilde{\tau}}} + \widetilde{n_\epsilon}\sqrt{\sigma_\epsilon^2\left(1-e^{-\frac{2\Delta t}{\tilde{\tau}}}\right)} \tag{5}$$

2.2 Master Equation

Master equation is an equation in quantum mechanical problems that used for open quantum system. The open system is a system in which there are interactions between the main quantum system and an environment around the system. The quantum state in the open system is represented by density matrix denoted by ρ. The density matrix represented the magnitude of probability distribution of quantum state $|\psi_n\rangle$. Representation of matrix ρ can be expressed by $\rho = \sum_n p_n|\psi_n\rangle\langle\psi_n|$ with p_n is a classical probability of the system at the state $|\psi_n\rangle$ [12]. If at the Hilbert space has been set an *arbitrary basis* $\{|\boldsymbol{i}\rangle\}_{\boldsymbol{i=1}}^{\boldsymbol{N}}$, so the density matrix of a quantum state can be expressed by [15]:

$$\rho = \sum_{i,j=1}^{N}\rho_{i,j}|i\rangle\langle j| = \begin{pmatrix}\rho_{00} & \rho_{01} & \cdots & \rho_{0N}\\ \rho_{10} & \rho_{11} & \cdots & \rho_{1N}\\ \vdots & \vdots & \ddots & \vdots\\ \rho_{N0} & \rho_{N1} & \cdots & \rho_{NN}\end{pmatrix} \tag{6}$$

In general, the master equation for the closed quantum system is expressed by [10, 12] ,

$$\dot{\rho}_{tot}(t) = -\frac{i}{\hbar}\big[H_{tot}(t), \rho_{tot}(t)\big] \tag{7}$$

Here, $\mathcal{H}_{tot}$ is the total Hamiltonian of the system summed up from the system Hamiltonian $\mathcal{H}_{sys}$, the environment Hamiltonian $\mathcal{H}_{env}$ and the interaction Hamiltonian $\mathcal{H}_{int}$, such that $\mathcal{H} = \mathcal{H}_{sys} + \mathcal{H}_{env} + \mathcal{H}_{int}$ [10]. In this study, the numerical calculation focuses on dynamics of the system, therefore the system density matrix ρ_s can be obtained by calculating it's trace from the total of density matrix ρ,

$$\rho_s = Tr_{env}[\rho] \tag{8}$$

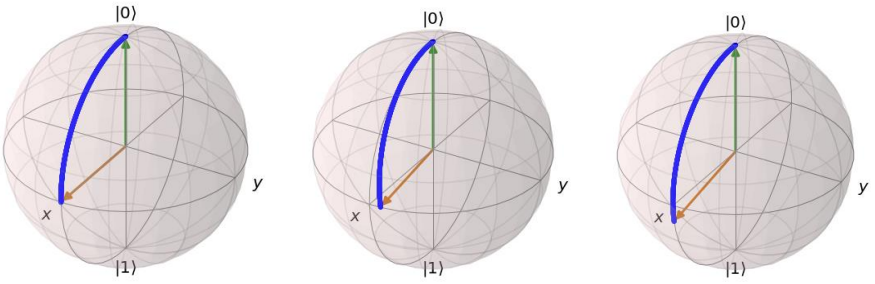
The calculation is continued by using Lindblad master equation with respect to the density matrix. This equation is used to perform calculations on an open quantum system,

$$\dot{\rho}(t) = -\frac{i}{\hbar}[\mathcal{H}(t), \rho(t)] + \sum_n \frac{1}{2}[2C_n\rho(t)C_n^\dagger - \rho(t)C_n^\dagger C_n - C_n^\dagger C_n\rho(t)] \tag{9}$$

with $C_n = \sqrt{\gamma_n} A_n$ are collapse operators, A_n are the operators through which the environment couples to the system in $\mathcal{H}_{int}$ and γ_n are the corresponding rates.

3. Results and Discussion

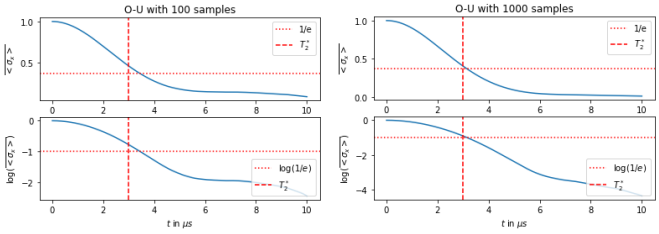
Here, we observe the dynamical of electron spin with and without errors or noises, as well as the decay process in form of Free Induction Decay (FID). For data retrieval, we vary the off – resonance error function if it equal to zero and not equal to zero ($\delta(t) = 0$ and $\delta(t) \neq 0$) so does with on - resonance error we also vary it to two conditions ($\epsilon(t) = 0$ and $\epsilon(t) \neq 0$). We set the total time $\pi/2$, $\Delta t = (\pi/2)/1000$, and $\phi = \pi/2$. This value of phi that affects the axis of rotation (will it rotate with respect to x, y, or z axis). Because of phi = $\boldsymbol{\frac{\pi}{2}}$, all of this data will rotate with respect to y – axis. The spin vector dynamics on the Bloch sphere is shown in Fig. 1.



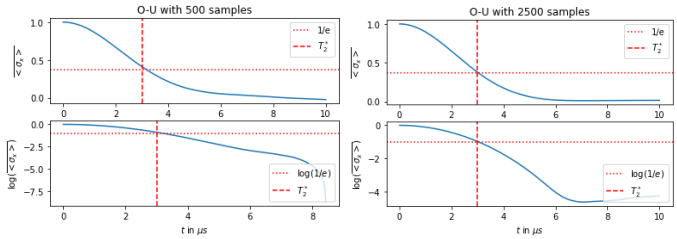
(a) (b) (c)

Figure 1. (a) Electron spin's rotation if there are no errors ($\delta(t) = 0$ and $\epsilon(t) = 0$) (b) Electron spin's rotation when there is off – resonance error ($\delta(t) \neq 0$) (c) Electron spin's rotation when there is on – resonance error $\epsilon(t) \neq 0$

Beside the affect of errors, we also want to observe the dynamical of the FID process and to prove that the spin magnetization relaxation time is $T_2^* = 3\mu s$ obtained from the typical experiment can be reproduced with the simulation using the OU process. At the simulation, we set the total time $t = 10\mu s$ with $\Delta t = 10\, ns$. We set the $\Delta t = 10\, ns$ in our simulation because we want to make it more realistic. In this case, for the experimental process, the tools named Arbitrary Waveform Generator can only reach out until 10 ns for doing the measurement. For initial state, we set the nuclear spin is in the superposition state $\left(\frac{|0\rangle+|1\rangle}{\sqrt{2}}\right)$. We vary the number of samples to 100, 500, 1000, and 2500 samples. The average expectation value along the x-axis for each variation of the OU samples is presented in Fig. 2. It is clearly shown that we obtained $T_2^* = 3\mu s$ if we use the OU sample as many as 2500.



(a) (c)



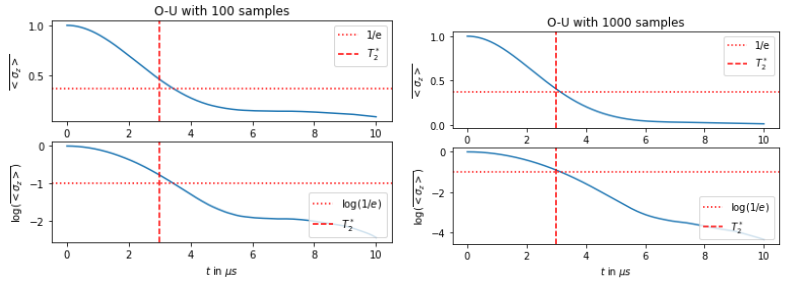
(b) (d)

Figure 2. Free Induction Decay Graph with expectation value at x-axis for (a) 100 samples, (b) 500 samples, (c) 1000 samples and (d) 2500 samples

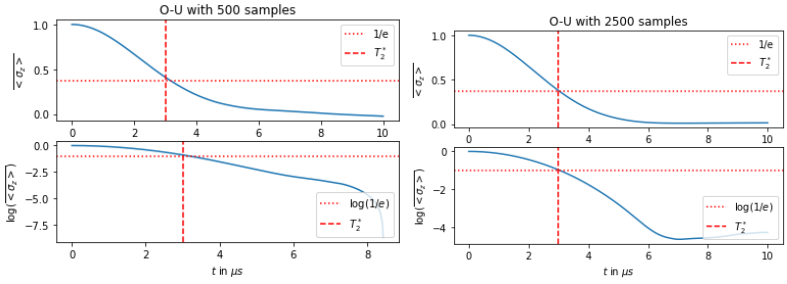
In Nitrogen – Vacancy centre system the decay from magnetisation spin of electron spin is only can be detected in the z – axis of Bloch sphere. To transform the decay process from x – axis to z – axis, we need to rotate the density matrix ρ for each time Δt, by applying a unitary operation called a $\pi/2$-rotation,

$$\rho(t) = U_1(t,0)\rho(t)U_1^{\dagger}(t,0) \tag{10}$$

The transformed dynamics is then obtained and presented in Fig. 3.



(a) (c)



(b) (d)

Figure 3. Free Induction Decay Graph with expectation value at z-axis for (a) 100 samples, (b) 500 samples, (c) 1000 samples and (d) 2500 samples

4. Conclusion

There are two types of error in the O-U process modelling, off-resonance error and on-resonance error. The off-resonance error makes the spin rotation tilted, because there is a detuning process. The on–resonance error cause the spin rotation to take a shorter or longer time. This time is also known as the controlling or rotation time. The ideal rotation for this problem is a rotation without

any noises or errors during the process. In this case, there is no control time and also without a detuning process. For magnetic resonance imaging, the decay process is in the form of free induction decay. The decay process causes the decoherence onthe magnetization spin. To detect the FID process in NV centre system, we need to rotate the electron spin to z-axis because NV centre system only can detect some measurements in z-axis. Hence, we need to transform the results to z-axis using the unitary evolution. Our simulations on the decoherence process of the NV electron spin using the Ornstein-Uhlenbeck process provide understanding for designing the building blocks of optimal control for nanoscale ESR and NMR in the presence of noise.

References

[1] Rieger P 2007 *Electron Spin Resonance* (The Royal Society of Chemistry)
[2] Kuzmany H 1998 *Solid-State Spectroscopy : An Introduction* (Springer Verlag) ISBN 9783540639138
[3] Schwart I, Rosskopf J, Schmitt S, Tratzmiller B, Chen Q, McGuiness L P, Jelezko F, Plenio M B 2019 *Scientific Reports*. **9** 6938
[4] Doherty M W, Dolde F, Fedder H, Jelezko F, Wratchrup J, Manson N B and Hollenberg L C L 2012 *Phys. Scientific Reports* B **85**(20) 205203
[5] Rembold P, Oshnik N, Muller M M., Montangero S, Calarco T, Neu E *AVS Quantum Science*. **2** 024701
[6] Bellac M 2006 *A short introduction to quantum information and quantum computation* (Cambridge University Press) ISBN 9781139457040
[7] Nielsen M and Chuang I 2010 *Quantum computation and quantum information: 10th anniversary edition* (Cambridge University Press) ISBN 9781139495486
[8] Hornak J 1996 *The Basics of NMR* (Rochester Institute of Technology, Centre for Imaging Space)
[9] Munera - Javaloy C, Puebla R, Casanova J 2021 *Europhysics Letters* **134** 30001
[10] Johansson J, Nation P, and Nori F 2013 *Computer Physics Communications* **184** 1234-1240
[11] Genov G T 2021 Ornstein – Uhlenbeck Numerical Simulation Note
[12] Manzano D 2020 *AIP Advances* **10** 025106