1. Introduction

A nitrogen-vacancy (NV$^-$) center in diamond [1–3] is a promising candidate to realize quantum information processing tasks [4–10]. An NV$^-$ center is known to have a long coherence time such as a second [11–13]. The operations such as qubit gates and measurements, which are basic tools for quantum applications, have been demonstrated with a single NV center [14]. Also, the entanglement generation between distant nodes, which plays an essential role of quantum repeater, has been demonstrated by using photons as flying qubits emitted through distant two single NV centers [15]. An NV$^-$ center can be used for a sensitive magnetic field sensor [16–18]. An ensemble of NV$^-$ centers can also be used for demonstrating quantum metrology [19–23] and physical phenomena in fundamental physics, such as quantum walk [24] and quantum simulation [25]. Also, the ensemble of NV$^-$ centers can be used as the hybrid devices between different physical systems, in particular, superconducting systems [26–38]. Due to the effect of a superradiance, the ensemble of NV$^-$ centers has a much stronger magnetic coupling with other systems than a single NV$^-$ center.

An NV$^-$ center consists of a nitrogen atom and a vacancy in the adjacent site [1], and this is a spin-1 system with three states of $|0\rangle$, $|\pm 1\rangle$, and $|1\rangle$. With a strong external magnetic field, the two exited states $|\pm 1\rangle$ of the NV$^-$ center is energetically separated far from each other. In this case, the NV$^-$ center can be considered as a spin $\frac{1}{2}$ system by using a frequency selectivity where $|0\rangle$ and $|1\rangle$ ($|\pm 1\rangle$) constitute a
The NV$^{-}$ center consists of a nitrogen atom (N) and a vacancy (V) in the adjacent site. Since the NV$^{-}$ center is a spin-1 system, we have three states of $|0\rangle$, $|1\rangle$, and $|-1\rangle$. We can characterize the NV$^{-}$ center by an optically detected magnetic resonance (ODMR) spectrum, and we perform the ODMR with an applied magnetic field of $B = 0, 1, 2$ mT, along the [111] direction.

Optically detected magnetic resonance (ODMR) is the general technique to investigate the properties of the NV$^{-}$ centers [2]. After applying a microwave pulse, the NV$^{-}$ centers are measured by an optical detection. Resonance observed with specific microwave frequencies let us know an energy structure of a ground-state manifold of the NV$^{-}$ centers. Also, we can estimate coherence properties of the NV$^{-}$ center from the width of the peaks.

Recently, a remarkably sharp dip has been observed around 2870 MHz in the ODMR with zero applied magnetic fields [29, 36, 42]. Although the ODMR results are usually fit by a sum of Lorentzians, the ODMR results observed in [29, 36, 42] cannot be well reproduced by such a fitting [29], and no theoretical model can explain the dip until a new approach is suggested in [36]. The model described in [36] contains spin-1 properties of the NV$^{-}$ centers while most of the previous models assume the NV$^{-}$ center to be a spin-half system or use just a sum of Lorentzians to include the effect of the spin-1 properties in a phenomenological way [29]. By including the strain distributions, randomized magnetic fields, and homogeneous width of the NV$^{-}$ centers, the sharp dip in the ODMR has been reproduced in [36]. This model provides us with an efficient tool to characterize the high-density ensemble of NV$^{-}$ centers, which would be crucial to realize diamond-based quantum information processing. Moreover, from the ODMR, we have estimated the strength of random magnetic field, strain variations, and homogeneous broadening of the NV$^{-}$ centers by using our model. To our best knowledge, this is the first report to estimate these parameters from the ODMR. In particular, the strain in diamond has an important role to manipulate the NV$^{-}$ center such as a mechanical spin control [43], an electric field interaction [41], generation of a spin squeezed state [44], and creation of a long-lived dark state [36]. So our technique to extract the information of the strain variations would play an important role to fabricate and characterize diamond-based devices for the realization of quantum information processing.

The rest of this paper is organized as follows. In section 2, we explain the experimental setup. In section 3, we introduce the theoretical model presented in [36]. In section 4, we show the ODMR results and explain how these experimental results can be reproduced by our theoretical model. Finally, section 5 contains a summary of our results.

2. Experimental setup

We begin by describing how we generate the NV$^{-}$ centers in diamond. To create the NV$^{-}$ center ensemble, we performed ion implantation of $^{12}$C$^{2+}$ and we annealed the sample in high vacuum [35]. The density of the NV$^{-}$ centers is approximately $5 \times 10^{17}$ cm$^{-3}$, and we have the NV$^{-}$ centers over the depth of 1 $\mu$m from the surface of the diamond.
The ODMR was performed on the diamond sample by a confocal microscope with a magnetic resonance system at room temperature [11]. The NV centers show spin-dependent fluorescence. When we illuminate green light on the NV centers, the NV centers are prepared in |0⟩ after a cyclic transition. Moreover, from the amount of emitted light, we can discriminate the state of |0⟩ and |±1⟩, which allows us to readout the spin state. Also, we can control the spin by microwave fields. We irradiated pulsed optical laser (532nm) and microwave independently to eliminate power broadening effect when we perform the ODMR. The magnetic field of 0, 1, or 2 mT was applied along the [111] axis. With zero or weak applied magnetic field, a quantization axis of the NV center is determined by the direction from the vacancy to the nitrogen, which we call an NV− axis. This axis is along one of four possible crystallographic axes. The NV− centers usually occupy these four directions equally. The applied magnetic field along [111] is aligned with one of these four axes as shown in figure 1. In this case, the Zeeman splitting of the NV− centers having the NV− axis of [111] is larger than that of the NV− centers having the other three NV− axes.

3. Model

We describe the model to simulate the ODMR of the NV− center ensemble, which was introduced in [36]. The NV− axis provides us with the z axis. Microwave pulses are applied on the NV− centers, and the microwave pulses orthogonal to the z axis induce the excitation of the NV− centers. We define the x axis as such a orthogonal direction of the applied microwave at each NV− center. The Hamiltonian of the NV− centers is as follows [45].

\[
H = \hbar \sum_{k=1}^{N} \left\{ D_k \hat{S}_{z,k}^2 + g_e \mu_B B_{zk}^e \hat{S}_{z,k} + E_1^{(k)} \left( \hat{S}_{x,k}^2 - \hat{S}_{y,k}^2 \right) + E_2^{(k)} \left( \hat{S}_{x,k} \hat{S}_{y,k} + \hat{S}_{y,k} \hat{S}_{x,k} \right) + \frac{\lambda}{2} \cos(\omega t) \hat{S}_{x,k}^{(k)} + \frac{\lambda}{2} \hat{S}_{z,k}^{(k)} + \frac{\lambda}{2} \left( \hat{S}_{x,k} \hat{I}_{z,k} - \hat{S}_{y,k} \hat{I}_{x,k} \right) + P \left( \hat{j}_{x,k} = \frac{\hbar}{2} \hat{j}_{y,k} - g_d \mu_B B_{zk}^d \hat{I}_{z,k} \right) \right\}
\]

where \( \hat{S}_{x,k} \) (\( \hat{I}_{z,k} \)) denotes a spin-1 operator of kth electron (nuclear) spin, \( D_k \) denotes a zero-field splitting, \( E_1^{(k)} \) (\( E_2^{(k)} \)) denotes a strain along x(y) direction, \( g_e \mu_B B_{zk}^e \). \( \hat{S}_{z,k} \) (\( -g_d \mu_B B_{zk}^d \)) denotes a Zeeman term of the kth electron (nuclear) spin, \( \lambda \) denotes a microwave amplitude, \( \omega \) denotes the microwave driving frequency, \( P \) denotes the quadrupole splitting, and \( \lambda_s \) (\( \lambda_p \)) denotes a parallel (orthogonal) hyperfine coupling. For simplicity, we assume a homogeneous microwave amplitude so \( \lambda_s \approx \lambda_p \). (In the appendix, we relax this constraint.) It is worth mentioning that the x and y component of the magnetic field is insignificant to change the quantized axis and so we consider only the effect of the z axis of the magnetic field. Since the energy of the nuclear spin is detuned from the energy of the electron spin, the flip-flop term \( \frac{\lambda}{2} \left( \hat{S}_{x,k} \hat{I}_{z,k} - \hat{S}_{y,k} \hat{I}_{x,k} \right) \) is negligible and the parallel term \( \frac{\lambda}{2} \hat{S}_{x,k}^{(k)} \) is dominant. In this case, the effect of the nuclear spin is considered as randomized magnetic fields on the electron spin [37, 38], and we can include this effect in the Zeeman splitting of the NV− centers. We use this approximation throughout the paper.

In a rotating frame defined by \( U = e^{-i \omega t} \hat{S}_{x,k}^{(k)} \), we can perform the rotating wave approximation giving the simplified Hamiltonian

\[
H \approx \hbar \sum_{k=1}^{N} \left\{ \left( D_k - \omega \right) \hat{S}_{z,k}^2 + E_1^{(k)} \left( \hat{S}_{x,k}^2 - \hat{S}_{y,k}^2 \right) + E_2^{(k)} \left( \hat{S}_{x,k} \hat{S}_{y,k} + \hat{S}_{y,k} \hat{S}_{x,k} \right) + \frac{\lambda}{2} \hat{S}_{z,k}^{(k)} + \frac{\lambda}{2} \left( \hat{S}_{x,k} \hat{I}_{z,k} - \hat{S}_{y,k} \hat{I}_{x,k} \right) \right\}
\]

where \( \hat{B}_{zk}(\hat{I}_{z,k}) \). 

The inhomogeneous broadening can be included in this model as follows. We use Lorentzian distributions to include an inhomogeneous effect of \( E_1^{(k)} \) and \( E_2^{(k)} \) \( (k = 1, 2, \ldots, N) \). It is worth mentioning that the Lorentzian distributions have been typically used to describe the inhomogeneous broadening of the NV− centers [35–37, 46]. For an inhomogeneous magnetic field \( B_{zk}^{(k)} \), we need to consider the following two effects. At first, since there is an electron spin-1/2 bath in the environment due to the substitutional N (P1) centers, NV− centers are affected by low frequency magnetic field noise. At second, a hyperfine coupling of the nitrogen nuclear spin splits the energy of the NV− center into three levels. So we use a random distribution of the magnetic fields with the form of the mixture of three Lorentzian functions. Here, each peak of the Lorentzian is separated with 2π × 2.3 MHz that corresponds to the hyperfine interaction with 14N nuclear spin [37, 38]. It is worth mentioning that, since the frequency shift of \( D_k \) is almost two-orders of magnitude smaller than that of \( E_1^{(k)} \) and \( E_2^{(k)} \) [41], we assume that the inhomogeneous width of zero field splitting is two orders of magnitude smaller than that of the strain in this paper.

It is worth mentioning that we can diagonalize the Hamiltonian described by equation (1), and this provides us with the information of the resonant frequency of the NV− centers as shown in [47]. However, such a diagonalization does not contain the information of the homogeneous broadening that comes from non-unitary dynamics between the NV− center and environment [2, 10, 48, 49]. Since the effect of the homogeneous broadening is relevant to reproduce our experimental results as we discuss later, we adopt the approach to solve a Lindblad master equation that includes such an environmental effect, which is different from the analysis in [47].

The Lindblad master equation at room temperature can be described as follows [10, 40, 49–53].
where $\gamma_{k,j} (j = 1, 2, 3, 4)$ denotes a decay rate and $\hat{L}_{k,j}(j = 1, 2, 3, 4)$ denotes a Lindblad operator on the $k$th NV $^\circ$. Here, $\hat{L}_{4,k} = |B\rangle_\delta^k \langle D|$ and $\hat{L}_{2,k} = |D\rangle_\delta^k \langle B|$ denote high frequency fluctuations of the magnetic field while $\hat{L}_{3,k} = |0\rangle_\delta^k \langle 0|$ and $\hat{L}_{6,k} = |D\rangle_\delta^k \langle 0|$ denote the energy relaxation. We set $\gamma_{1,k} = \gamma_{2,k} = \Gamma$ as the dephasing rate of the high frequency magnetic field noise and set $\gamma_{3,k} = \gamma_{4,k} = \gamma_{6,k} = \Gamma$ as the energy relaxation rate. However, it is difficult to solve this master equation analytically. So we consider a simplified master equation described as follows.

$$\frac{d\rho(t)}{dt} = -\frac{i}{\hbar}[H, \rho(t)] + \sum_{k=1}^{N} \sum_{j=1}^{4} \gamma_{k,j} \hat{L}_{k,j} \rho(t) \hat{L}_{k,j}^\dagger - \rho(t) (\hat{L}_{k,j}^\dagger \hat{L}_{k,j}) \quad (2)$$

where we ignore the thermal effect described by the Lindblad operators of $\hat{L}_{3,k}$ and $\hat{L}_{6,k}$. Strictly speaking, the solution of the equation (3) should be different from the solution of the equation (2) if the thermal effect is relevant. Fortunately, since the thermalization rate is much smaller than other parameters such as a dephasing rate, we measure the NV centers by a laser before we start observing the thermalization effect in the ODMR. In this case, we can take a limit of a small $\Gamma^\prime$ so that the solution of equation (3) should coincide with the solution of the equation (2).

We will describe how we can obtain an analytical solution of the master equations. We assume that the driving strength $\lambda$ is much smaller than other parameters to avoid a power broadening in the spectrum [54]. Since we consider a steady state after a long time, we can set the time derivative as zero. In these conditions, we obtain the probability for the NV $^\circ$ center to be in the $|0\rangle$ state by solving the master equation of equation (3) as follows.

$$P_0 = 1 - \frac{1}{N} \text{Tr}[\rho(\infty) \sum_{k=1}^{N} |0\rangle_\delta^k \langle 0|] = 1 - \frac{1}{N} \left( \sum_{k=1}^{N} \frac{\lambda^2 (\omega - \omega_b^{(k)} + i \Gamma^\prime)}{\left(\omega - \omega_b^{(k)} + i \Gamma^\prime\right)^2 - (|J_k|^2 + |J_k^d|^2)} \right)$$

(4)

where we define $\omega_b^{(k)} = D_k - E_1^{(k)}$, $\omega_d^{(k)} = D_k + E_1^{(k)}$, $J_k = g \mu_B B_k^z$, $J_k^d = E_2^{(k)}$, $\Gamma^\prime = \Gamma + \gamma$, and $\lambda = \frac{\Gamma^\prime}{\sqrt{\Gamma^\prime} \lambda}$. We can take a limit of a small energy decay rate $\Gamma^\prime$ in equation (4) while we keep the effective driving strength $\lambda = \frac{\Gamma^\prime}{\sqrt{\Gamma^\prime} \lambda}$ as a constant. So we obtain

$$P_0 \approx 1 - \frac{1}{N} \left( \sum_{k=1}^{N} \frac{\lambda^2 (\omega - \omega_b^{(k)} + i \Gamma^\prime)}{\left(\omega - \omega_b^{(k)} + i \Gamma^\prime\right)^2 - (|J_k|^2 + |J_k^d|^2)} \right) + \left| \frac{\lambda (J_k^d - J_k)}{(\omega - \omega_b^{(k)} + i \Gamma^\prime)(\omega - \omega_b^{(k)} + i \Gamma^\prime) - (|J_k|^2 + |J_k^d|^2)} \right|^2$$

(5)

and this corresponds to the solution of the master equation of the equation (2).

In the actual experiment, if we excite the NV $^\circ$ centers by the microwave pulses, the intensity of the photons emitted from the NV $^\circ$ centers will be changed from the baseline emission rate $I_0$. This change is linear with $(1 - P_0)$. So, to fit the experiment with our model, we use a function of $(I_0 - a (1 - P_0))I_0$ where $a$ denotes a fitting parameter, and this corresponds to the ODMR signals.

4. Experimental results and theoretical fitting

By using the model described above, we have reproduced the ODMR signals when we apply $B = 0, 1, 2$ mT, as shown in figures 2–4. For the case of $B = 0$ mT, the microwave transitions from the ground state to the excited states are largely suppressed around 2870 MHz where the ODMR intensity becomes close to the baseline, and we call this a sharp dip. Our simulation can reproduce this. Two peaks are observed in the ODMR with zero applied magnetic field as shown in figure 2, which corresponds to the transition between state $|0\rangle$ and one of the other energy eigenstates. If we consider a single NV $^\circ$ center, the frequency difference between the two exited states is $\delta \omega = 2\sqrt{(g \mu_B B)^2 + (E_1)^2 + (E_2)^2}$. Since we consider an ensemble of the NV $^\circ$ center, this frequency difference varies depending on the position of the NV $^\circ$ center. For simplicity, we use a dimensionless variable for $B$, $E_1$, and $E_2$, defined as $B_z = g \mu_B B_z/\gamma$, $E_1 = E_1/\gamma$, and $E_2 = E_2/\gamma$ where $\gamma$ denotes a damping rate with a unit of the frequency. To calculate a probability that the two energy eigenstates such as $|1\rangle$ and $|-1\rangle$ are degenerate ($\delta \omega = 0$), we define probability density functions of $\tilde{B}_z$, $\tilde{E}_1$, and $\tilde{E}_2$ as $P_0(\tilde{B}_z)$, $P_0(\tilde{E}_1)$, and $P_0(\tilde{E}_2)$, respectively. The joint probability is calculated as

$$P_0(\tilde{B}_z, \tilde{E}_1, \tilde{E}_2) \Delta \tilde{B}_z \Delta \tilde{E}_1 \Delta \tilde{E}_2 = P_0(\tilde{B}_z = 0) \Delta \tilde{B}_z \cdot P_0(\tilde{E}_1 = 0) \Delta \tilde{E}_1 \cdot P_0(\tilde{E}_2 = 0) \Delta \tilde{E}_2.$$
where $\hat{B}_i = r \sin \theta \cos \phi$, $\hat{E}_i = r \sin \theta \sin \phi$, $\hat{E}_2 = r \cos \theta$ with $r = \sqrt{\hat{B}_1^2 + \hat{E}_1^2 + \hat{E}_2^2}$, we rewrite this as

$$P(\hat{B}_1, \hat{E}_1, \hat{E}_2) \Delta \hat{B}_1 \Delta \hat{E}_1 \Delta \hat{E}_2 = P(\hat{B}_1 = 0)P(\hat{E}_1 = 0)P(\hat{E}_2 = 0)r^2 \sin \theta \Delta \theta \Delta \phi.$$  

This shows that, even if we consider a finite range $\Delta \hat{B}_1$, $\Delta \hat{E}_1$, and $\Delta \hat{E}_2$, the probability for the two energy eigenstates to be exactly degenerate ($r = 0$) is zero. This means that, if homogeneous broadening is negligible, the two peaks to denote the two energy eigenstates of each NV$^-$ center should always be separated in the ODMR so that the ODMR signal at the frequency of $D/2\pi = 2870$ MHz should be the same as the base line. However, due to the effect of the homogeneous broadening, small signals deviated from the base line can be observed at the frequency of $D/2\pi = 2870$ MHz. This is the cause of the sharp dip observed around the frequency of $2\pi \times 2870$ MHz in the ODMR. It is worth mentioning that, although we reproduced the ODMR without applied magnetic field by using a numerical simulation, we did not discuss the physical origin of the sharp dip in [36]. In this paper, we firstly find out the mechanism why such a sharp dip appears in the ODMR with an analytical calculation, as explained above.

With an applied magnetic field, four peaks are observed in the ODMR where two of them are larger than the other two, as shown in figures 3 and 4. The two smaller peaks correspond to the energy eigenstates of the NV$^-$ centers with a NV$^-$ axis along [111], which is aligned with the applied magnetic field. A quarter of the NV$^-$ centers in the ensemble have such a NV$^-$ axis. The other larger peaks come from the other NV$^-$ centers where the applied magnetic field is not aligned with the NV$^-$ axis. Three-quarters of the NV$^-$ center have such axes. In this case, the Zeeman splitting of these is smaller than that of the NV$^-$ centers with the [111] axis. It is worth mentioning that a small dip is observed in the 1 mT ODMR around $2\pi \times 2870$ MHz due to the mechanism explained above. On the other hand, such a dip is not clearly observed in the 2 mT ODMR, because the NV$^-$ centers are considered to be as approximate two-level systems in this regime.

5. The sensitivity of ODMR to core system parameters

We perform numerical simulations with several parameters to understand the behavior of the sharp dip with zero applied magnetic fields. In figure 5(a), we change the parameter $\Gamma$ while we fix the other parameters. Similarly, we change the parameter $\delta B_k (\delta E_k)$ while we fix the other parameters. We have found that the sharp dip is very sensitive against the change in $\Gamma$ as shown in figure 5(a). On the other hand, we have confirmed that the dip is insensitive against the change in $\delta E_k$ and $\delta B_k$.

Also, we perform numerical simulations with several parameters for the ODMR with an applied magnetic field. In figure 5(b), we have plotted one of the peaks of the ODMR with an applied magnetic field of 2 mT. This peak corresponds to a transition between $|0\rangle$ and $|\pm 1\rangle$ of the NV$^-$ center with an axis of [111].

From the numerical simulations, we have found that this ODMR signal with applied magnetic field is robust against the strain variations $\delta E_k$, while the peak will be broadened due to the effect of the randomized magnetic field $\delta B_k$. The frequency difference between the ground state and another energy eigenstate can be calculated as

\[ \Delta \omega = \left( \frac{g \mu_B B}{\hbar} \right) \delta B_k \]

Figure 2. ODMR with zero applied magnetic fields. $\delta (g \mu_B B)/2\pi = 1.96$ MHz (HWHM), $\delta E_1/2\pi = \delta E_2/2\pi = 0.73$ MHz (HWHM), $\delta D_k = 0.01$ MHz (HWHM), $\lambda/2\pi = 2$ MHz, $\Gamma/2\pi = 0.3$ MHz. Also, we assume a nitrogen hyperfine coupling of $2\pi \times 2.3$ MHz. The red line denotes a numerical simulation and blue dots denote the experimental results.

Figure 3. ODMR with an applied magnetic field of 1 mT. We use the same parameters as figure 2. The red line denotes a numerical simulation and blue dots denote the experimental results.

Figure 4. ODMR with an applied magnetic field of 2 mT. We use the same parameters as figure 2. The red line denotes a numerical simulation and blue dots denote the experimental results.
\[ \delta \omega' = D_k - \sqrt{E_1^{(k)} + E_2^{(k)} + (g_e\mu_B B_z^{(k)})^2}. \]

If the applied magnetic field is large, we obtain \( \delta \omega' \approx g_e\mu_B B_z^{(k)} \). This means that the effect of the strain is insignificant in this regime while the inhomogeneous magnetic field from the environment can easily change this frequency. These can explain the simulation results shown in figure 5(b) where the change of inhomogeneous magnetic fields affects the width of the peak. On the other hand, we have confirmed that the peak width is insensitive against the inhomogeneous strain. Such an effect to suppress the strain distributions by an applied magnetic field was mentioned in [55], and was recently demonstrated in a vacuum Rabi oscillation between a superconducting flux qubit and NV− centers in [56]. Our results here are consistent with these previous results.

6. Parameter estimation

An ensemble of NV− centers is mainly affected by inhomogeneous magnetic fields, inhomogeneous strain distributions, and homogeneous broadening. In the ODMR, the observed peaks contain the information of the total width that is a composite effect of the three noises mentioned above, and so it was not straightforward to separate these three effects for the estimation of how individual noise contributes to the width.

Here, we explain how we have estimated the parameters to reproduce the experimental results by using our model. Firstly, as we described before, the sharp dip in the ODMR is very sensitive against the change in \( \Gamma \), while the dip is relatively insensitive against the change in \( \delta E_k \) and \( \delta B_k \). These properties are important to determine the value of \( \Gamma \) from the analysis of the ODMR. Usually, \( \Gamma \) is much smaller than the \( \delta B_k \) and \( \delta E_k \) [35, 36, 38, 56], and so it seems that the effect of \( \Gamma \) might be hindered by a huge influence of \( \delta B_k \) and \( \delta E_k \). However, since the dip is sensitive against the change in \( \Gamma \), we could accurately estimate the \( \Gamma \) even under the effect of \( \delta B_k \) and \( \delta E_k \). Secondly, as we have shown, the ODMR signal with applied magnetic field is robust against the strain variations \( \delta E_k \) while the peak will be broadened due to the effect of the randomized magnetic field \( \delta B_k \). We can use these properties to estimate the \( \delta B_z^{(k)} \) and \( \delta E_k \). Since the ODMR with an applied magnetic field is insensitive against \( \delta E_k \), we can estimate \( \delta B_z^{(k)} \) from this experimental data. Since we have estimated \( \delta B_z^{(k)} \) and \( \Gamma \) from the prescription described above, we fix these parameters so that we can estimate \( \delta E_k \) from the ODMR with zero applied magnetic field. Therefore, by applying these procedures, we can estimate the parameters of the NV− centers such as inhomogeneous magnetic fields, inhomogeneous strain distributions, and homogeneous broadening. To our best knowledge, this is the first report to estimate these parameters from the ODMR.

7. Summary

In conclusion, we have studied an ODMR with a high-density ensemble of NV− centers. Our model succeeds in reproducing the ODMR with and without applied magnetic field. Also, we have explained how we can use our model to estimate the typical parameters of the ensemble NV− centers such as strain distributions, inhomogeneous magnetic fields, and homogeneous broadening width. Such a characterization is essential for the use of NV− centers to realize diamond-based quantum information processing.

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Appendix

Here, we consider the effect of inhomogeneous microwave amplitude. As described in equation (5), the probability of obtaining a ground state is as follows:

\[
P_0 = 1 - (P_b + P_d)
\]

\[
P_b = \frac{1}{N} \sum_{k=1}^{N} \left( \omega - \omega_b^{(k)} + i \Gamma_b \right) (\omega - \omega_d^{(k)} + i \Gamma_d) - (|J_b|^2 + |J_d|^2)^2
\]

\[
P_d = \frac{1}{N} \sum_{k=1}^{N} \left( \omega - \omega_b^{(k)} + i \Gamma_b \right) (\omega - \omega_d^{(k)} + i \Gamma_d) - (|J_b|^2 + |J_d|^2)^2
\]

where the value of \( \lambda \) differs depending on the position of the NV\(^-\) centers. Since inhomogeneity of \( \lambda \) is independent from the inhomogeneity of \( \omega_b, \omega_d, J_b \), and \( J_d \), we can rewrite these probabilities for a large number of NV\(^-\) centers as follows:

\[
P_b \approx \frac{1}{N} \sum_{j=1}^{m} \left( \lambda \right)^2 \sum_{k=1}^{N} p_k^{(b)} = \left( \frac{1}{N} \sum_{j=1}^{m} \left( \lambda \right)^2 \sum_{k=1}^{N} p_k^{(b)} \right)
\]

\[
P_d \approx \frac{1}{N} \sum_{j=1}^{m} \left( \lambda \right)^2 \sum_{k=1}^{N} p_k^{(d)} = \left( \frac{1}{N} \sum_{j=1}^{m} \left( \lambda \right)^2 \sum_{k=1}^{N} p_k^{(d)} \right)
\]

Therefore, we obtain

\[
P_b \approx |\lambda||^2 \frac{1}{N} \sum_{k=1}^{N} p_k^{(b)}
\]

\[
P_d \approx |\lambda||^2 \frac{1}{N} \sum_{k=1}^{N} p_k^{(d)}
\]

where \( |\lambda||^2 = \frac{1}{N} \sum_{j=1}^{m} |\lambda||^2 \) and \( N = \text{floor}(N) \). The probability of the NV\(^-\) center in the ground states can be calculated as

\[
P_0^g = 1 - (P_b + P_d)
\]

and this is the same form as the probability of the homogeneous microwave amplitude case described in the equation (5) where \( N (\lambda^2) \) is replaced by \( N'(\lambda^2) \). So the inhomogeneous microwave amplitude does not affect the theoretical prediction of ODMR signals.

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