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Dynamics of the Overhauser field under nuclear spin diffusion in a quantum dot

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Abstract. The coherence of electron spins can be enhanced significantly by preparing the nuclear spin polarizations to generate an Overhauser field with small fluctuations. We propose a theoretical model for calculating the long time dynamics of the prepared Overhauser field under nuclear spin diffusion in a quantum dot. We obtained a simplified diffusion equation that can be numerically solved, and we show quantitatively how the Knight shift and the electron-mediated nuclear spin flip-flops affect the nuclear spin diffusion. The results explain several recent experimental observations, where the measured decay time of the Overhauser field is dependent on the external magnetic field, electron spin state in double quantum dots and initial nuclear spin polarization rate.

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1. Introduction

Electron spins in quantum dots are one of the most promising systems for realizing quantum computation [1]. The spin state of a single electron in a quantum dot can be coherently controlled either optically through fast laser pulses or electronically by tuning gate voltages [1]–[5]. In experiments, the coherence time of the electron spin is largely limited by its hyperfine coupling to the nuclear spin environment in the host semiconductor material. The coupling causes spectral diffusion and gives a typical spin decoherence time of $T_2^* \sim 15$ ns for the electron spin qubit [6, 7]. This coherence time could be significantly prolonged with the application of spin echo [8] or other dynamic decoupling techniques (see [9] and references therein). However, implementation of these techniques requires the repeated application of many laser pulses. Each pulse inevitably induces some noise by itself, which limits the practical performance of suppressing spin noise under real environments.

Another technique for increasing the coherence time of the electron spin is dynamic nuclear spin polarization (DNP) [10]–[20], which prepares the nuclear spin environment into certain configurations. The nuclear spins in such configurations collectively generate an effective magnetic field (the Overhauser field) on the electron spin with small fluctuations, hence decreasing the spectral diffusion of the electron spin. Although nuclear spins can be polarized by many methods such as optical pumping [10], a substantial reduction in the fluctuation of the Overhauser field requires almost complete polarization of the nuclear spins [21], which is hard to achieve experimentally. Recent experiments, including both optically and electronically controlled quantum dot systems [13]–[16], however, demonstrate surprising feedback mechanisms that can lock the Overhauser field to certain values without significant polarization of the nuclear spins. The Overhauser field generated from such a locking mechanism has much smaller fluctuation, which effectively increases the coherence time T_2^* of the electron spin qubit by up to two orders of magnitude.

The DNP process prepares a fixed Overhauser field with small fluctuations that enables us to perform gate experiments on the electron spins over a longer coherence time. Important questions under this background are: How long can this fixed Overhauser field survive after the DNP process and what factors determine/influence the relaxation time of the Overhauser field? Recent experiments have revealed that the Overhauser field has a typical relaxation time ranging from a few seconds to a few minutes, and even up to an hour in certain systems [22]. The variation of this relaxation time is believed to be a result of diverse experimental configurations, such as different applied magnetic fields [18, 19], electron spin state in double quantum dots [18] and DNP pump time [20].

In this paper, we develop a quantitative theory for calculating the relaxation time of the Overhauser field in the environment of quantum dots, and provide a qualitative explanation of the dependence of the Overhauser field relaxation time on various experimental configurations mentioned above. The relaxation of the Overhauser field is widely believed to be caused by nuclear spin diffusion. In bulk material, nuclear spin diffusion has been well studied [23, 24] and is caused simply by the nuclear dipole–dipole interaction. In a quantum dot, however, the presence of the electron spin generates two new effects in the diffusion process. Firstly, the electron spin can mediate the diffusion of nuclear spins through a virtual hyperfine process. Secondly, the effective magnetic field generated by the polarized electron spin produces an inhomogeneous Knight shift on the surrounding nuclear spins, and this Knight shift can suppress the nuclear spin diffusion. The influence of the Knight shift on the nuclear spin diffusion

coefficient has been taken into account in [25], but electron-mediated nuclear spin diffusion was ignored there. Without considering electron-mediated diffusion, one cannot explain the dependence of the Overhauser field relaxation time on various experimental parameters such as the magnetic field. A more recent work [26] considers relaxation of the Overhauser field due to the electron-mediated nuclear spin diffusion, but not including the direct nuclear dipole–dipole interaction. Such treatment ends up with the conclusion that the Overhauser field can only decay by less than 1%, in contrast to experimental facts of complete decay of the Overhauser field over a long time. A quantitative theory that includes a complete description of both effects is, to our knowledge, still lacking. In this work, we take into account both electron-mediated nuclear spin diffusion and direct nuclear dipole–dipole diffusion, and the results are consistent with the recent experimental observations in [18]–[20].

The paper is organized as follows. In section 2, we give a formalism for describing relaxation of the Overhauser field that includes contributions from the nuclear dipole–dipole interaction, the electron-mediated nuclear spin diffusion and the Knight shift. Then we derive the effective nuclear spin diffusion equation and solve it numerically to determine the relaxation time of the Overhauser field. In section 3, we compare our calculation results with the recent experiments and show that they are in qualitative or semi-quantitative agreement. We summarize our results in section 4 with brief discussions.

2. Decay of the Overhauser field through nuclear spin diffusion

We assume that an external magnetic field B_0 much larger than the mean value and variance of the local Overhauser field generated by nuclei is applied along the z -direction (perpendicular to the quantum dot layer). In this case, we can drop the nonsecular terms in the interaction Hamiltonian [27]. For simplification, we consider only one species of nuclei around the quantum dot electron. The total Hamiltonian for the electron and nuclear spin systems, including both the Fermi contact hyperfine interaction and nuclear dipole–dipole interaction, can be written as

$$H = H_e + H_n + H_{en} + H_{nn}, \quad (1)$$

$$H_e = -g_e \mu_B B_0 S^z, \quad (2)$$

$$H_n = -g_n \mu_N B_0 \sum_i I_i^z, \quad (3)$$

$$H_{en} = \sum_i A_i S^z I_i^z + \sum_i \frac{A_i}{2} (S^+ I_i^- + S^- I_i^+), \quad (4)$$

$$H_{nn} = \sum_{i \neq j} 2B_{ij} I_i^z I_j^z - \sum_{i \neq j} B_{ij} I_i^+ I_j^-, \quad (5)$$

$$B_{ij} = \frac{\mu_0}{4\pi} (g_n \mu_N)^2 R_{ij}^{-3} (1 - 3 \cos^2 \theta_{ij}), \quad (6)$$

where A_i denotes the hyperfine coupling between the electron and nuclear spins at site i with spatial coordinates (x_i, y_i, z_i) . R_{ij} is the distance between two nuclei at site i, j . θ_{ij} is the angle between the line connecting sites i, j and the z -direction.

We note that for B_0 ranging from a few mT to a few T, the electron's Zeeman splitting is of the order of 10^{-1} – 10^2 GHz, while the average hyperfine coupling in most quantum dot systems

is of the order of MHz. Thus we can adiabatically eliminate the spin-flip terms in the hyperfine interaction Hamiltonian and correspondingly modify the other terms in the Hamiltonian as [26]

$$H_e = - \left(g_e \mu_B B_0 + \frac{\sum_i A_i^2}{4g_e \mu_B B_0} \right) S^z, \quad (7)$$

$$H_n = \sum_i \left[-g_n \mu_N B_0 + A_i \left(1 - \frac{A_i}{4g_e \mu_B B_0} \right) S^z \right] I_i^z, \quad (8)$$

$$H_{nn} = \sum_{i \neq j} 2B_{ij} I_i^z I_j^z - \sum_{i \neq j} \left(B_{ij} + \frac{A_i A_j S^z}{2g_e \mu_B B_0} \right) I_i^+ I_j^-, \quad (9)$$

where we have introduced an electron-mediated nuclear flip-flop term in H_{nn} . Since we are interested in the long time dynamics of nuclear spins, we can completely eliminate the electron from the Hamiltonian by replacing the constant operator S^z with its expectation value. We find that using $S^z = 1/2$ or $S^z = -1/2$ will yield almost the same result in the following calculations. Therefore, we can set $S^z = 1/2$ for simplicity and arrive at the following effective Hamiltonian (neglecting constant terms):

$$H = H_0 + H_1, \quad (10)$$

$$H_0 \approx \sum_i (-g_n \mu_N B_0 + A_i/2) I_i^z + \sum_{i \neq j} 2B_{ij} I_i^z I_j^z, \quad (11)$$

$$H_1 = - \sum_{i \neq j} \left(B_{ij} + \frac{A_i A_j}{4g_e \mu_B B_0} \right) I_i^+ I_j^-. \quad (12)$$

Here, the term proportional to A_i in H_0 is the Knight shift term. For this Knight shift, we have neglected the small term proportional to A_i^2 in equation (8) as it is dominated by the A_i term in most experimental systems.

The expectation value for the z -component of nuclear spin at site k will evolve according to the Schrödinger equation:

$$\frac{\partial \langle I_k^z \rangle}{\partial t} = \frac{i}{\hbar} \text{Tr}\{\rho(t)[H_1, I_k^z]\}, \quad (13)$$

where $\rho(t)$ is the nuclear spin density matrix at time t , which can be calculated by switching to the interaction picture:

$$\tilde{\rho}(t) = \rho(0) + \frac{i}{\hbar} \int_0^t [\tilde{\rho}(t'), \tilde{H}_1(t')] dt', \quad (14)$$

with $\tilde{H}_1(t) = \exp(iH_0 t/\hbar) H_1 \exp(-iH_0 t/\hbar)$. Further calculation yields [23]

$$\frac{\partial \langle I_k^z \rangle}{\partial t} = \frac{i}{\hbar} \text{Tr}\{\rho(0)[\tilde{H}_1(t), I_k^z]\} + \left(\frac{i}{\hbar} \right)^2 \int_0^t \text{Tr}\{\rho(t-t')[H_1, [\tilde{H}_1(t'), I_k^z]]\} dt'. \quad (15)$$

We assume the nuclear spin (with spin- I) density matrix to be a product state of the following form:

$$\rho(t) = \bigotimes_k \rho_k(t), \quad \rho_k(t) = \frac{1}{2I+1} + \frac{\langle I_k^z(t) \rangle}{\text{Tr}\{(I_k^z)^2\}} I_k^z. \quad (16)$$

Such an approximation is valid when off-diagonal terms of the density matrix are negligible. This is justified by the fact that fluctuations in B_0 and inhomogeneous Knight shift will quickly destroy correlation and transverse coherence between the nuclear spins [26, 28]. Besides, calculating without this approximation will not change the physical nature of the result, as the authors of [23] have shown that off-diagonal terms only have a minor contribution to the diffusion coefficients.

By using the explicit form of the Hamiltonian (equations (10)–(12)) and the density matrix (equation (16)), equation (15) reduces to

$$\frac{\partial \langle I_k^z \rangle}{\partial t} = \sum_{i \neq k} W_{ik} (\langle I_i^z(t) \rangle - \langle I_k^z(t) \rangle), \quad (17)$$

$$W_{ki} = \frac{1}{\text{Tr}\{(I_k^z)^2\}} \int_0^t \text{Tr}\{[\tilde{H}_1(t), I_k^z][\tilde{H}_1(t-t'), I_i^z]\} dt',$$

where W_{ki} has a clear physical meaning as the flip-flop rate between nuclear spins at sites i and k .

For a two-dimensional (2D) InAs/GaAs quantum dot, we take As nuclei ($I = 3/2$) as an example for further calculation. The parameter W_{ki} can be analytically calculated when approximating the integration upper limit in the above expression for W_{ki} from t to infinity [25].

$$W_{ik} = \frac{17\sqrt{2\pi}}{5} C_{ik}^2 (A_{ik}^2 + g_{ik})^{-1/2} + \frac{12\sqrt{2\pi}}{5} C_{ik}^2 (A_{ik}^2 + 64C_{ik}^2 + g_{ik})^{-1/2} \\ + \frac{9\sqrt{2\pi}}{10} C_{ik}^2 (A_{ik}^2 + 256C_{ik}^2 + g_{ik})^{-1/2}, \quad (18)$$

$$A_{ik} = A_i - A_k, \quad (19)$$

$$C_{ik} = B_{ik} + \frac{A_i A_k}{4g_e \mu_B B_0}, \quad (20)$$

$$g_{ik} = 80 \sum_{j \neq i, k} (C_{ij} - C_{kj})^2. \quad (21)$$

The hyperfine coupling rate A_i is proportional to the square of the electron wave function in a quantum dot. In the following calculation, we assume that the dot potential is like a square well in the z -direction and the electron wave function takes a Gaussian shape in the x, y -plane. The hyperfine coupling rate A_i can then be written as $A_i = A_0 \cos^2(\pi z_i/z_0) \exp[-(x_i^2 + y_i^2)/l_0^2]$, where (x_i, y_i, z_i) are spatial coordinates of site i . l_0 and z_0 are, respectively, the Fock–Darwin radius and thickness of the quantum dot, and A_0 is the hyperfine coupling for the nuclear spin at the origin (electron's location).

The assumption that the nuclear spins follow a diffusion process requires the flip-flop rate for two distant sites to be negligible. This requirement is satisfied by the fact that the coefficient C_{ik} decays to zero fast as R_{ik} increases ($B_{ik} \propto R_{ik}^{-3}$ and $A_i A_k \leq A_0 \exp[-(R_i^2 + R_k^2)/l_0^2] \leq A_0 \exp(-R_{ik}^2/l_0^2)$, where we ignore the diffusion in the z -direction as discussed below). If we treat $\langle I_k^z(t) \rangle$ as a continuous function of the spatial variable x^α ($\alpha = x, y, z$), we can then carry out a Taylor expansion of $\langle I^z(t) \rangle$ for site i around site k :

$$\langle I_i^z(t) \rangle \approx \langle I_k^z(t) \rangle + \frac{\partial \langle I_k^z(t) \rangle}{\partial x^\alpha} (x_k^\alpha - x_i^\alpha) + \frac{1}{2} \frac{\partial^2 \langle I_k^z(t) \rangle}{\partial x^\alpha \partial x^\beta} (x_k^\alpha - x_i^\alpha)(x_k^\beta - x_i^\beta) + \dots, \quad (22)$$

where Einstein's summation convention is implied for the spatial index α, β . Substituting this into equation (17) and noting that the summation of the first-order derivative term over all sites vanishes due to the lattice symmetry⁴, we have

$$\frac{\partial \langle I_k^z \rangle}{\partial t} \approx \left[\sum_{i \approx k} \frac{1}{2} W_{ik} (x_k^\alpha - x_i^\alpha)(x_k^\beta - x_i^\beta) \right] \frac{\partial^2 \langle I_k^z(t) \rangle}{\partial x^\alpha \partial x^\beta}. \quad (23)$$

The $\sum_{i \approx k}$ notation above means summarization over the sites near k . Define the coefficient $D^{\alpha\beta} = \sum_{i \approx k} W_{ik} (x_k^\alpha - x_i^\alpha)(x_k^\beta - x_i^\beta)/2$ and similarly note that for $\alpha \neq \beta$ the summation over all sites vanishes; we have

$$\frac{\partial \langle I_k^z \rangle}{\partial t} = \left(D^{xx} \frac{\partial^2}{\partial x^2} + D^{yy} \frac{\partial^2}{\partial y^2} + D^{zz} \frac{\partial^2}{\partial z^2} \right) \langle I_k^z(t) \rangle. \quad (24)$$

Equation (24) is a 3D anisotropic diffusion equation with spatially varying diffusion coefficients (as A_{ik} , B_{ik} and W_{ik} all depend on the spatial coordinates), which is not easy to solve. To further simplify it, we note that to obtain the major feature for the full-time dynamics of the Overhauser field $\langle h_z(t) \rangle = \sum_k A_k \langle I_k^z(t) \rangle$, it is reasonable to first ignore the diffusion in the z -direction, because the quantum dot layer is usually a few nm thick and chemical or structural mismatch in adjacent layers can strongly suppress diffusion in the z -direction [19]. In addition, from symmetry in the 2D x, y -plane, we expect to have $D^{xx} \approx D^{yy}$ and can thus define an average 2D diffusion coefficient $D(x, y) = \sum_{i \approx k} W_{ik} [(x_k - x_i)^2 + (y_k - y_i)^2]/4$. Now we have a simplified 2D diffusion equation:

$$\frac{\partial \langle I_k^z \rangle}{\partial t} = D(x, y) \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) \langle I_k^z(t) \rangle. \quad (25)$$

The above partial differential equation can be effectively solved using the finite-element method by coarse graining a large number of nuclear spin sites to a small number of mesh nodes. But before solving equation (25), we would like to have some discussion about the diffusion coefficient $D(x, y)$. For $x, y \gg l_0$, the role of electrons can be neglected and a numerical calculation of the above diffusion coefficient gives a uniform background value $D \approx 7 \text{ nm}^2 \text{ s}^{-1}$, consistent with previous theoretical and experimental reports on the diffusion coefficient in bulk material [23]–[25]. In our calculation, we set the quantum dot parameters $l_0 = 30 \text{ nm}$, $z_0 = 10 \text{ nm}$, $A_0 = 1 \mu\text{eV} \approx 1.5 \text{ MHz}$, $\sum_k A_k \approx 80 \mu\text{eV}$, the lattice constant $a_0 = 0.563 \text{ nm}$ and the number of nuclei $N \approx 9 \times 10^5$, according to typical experimental values [17]–[19].

Within the range of the Fock–Darwin radius l_0 , the presence of the quantum dot electron will change the diffusion coefficient through two competing mechanisms: on the one hand, the confined electron generates an inhomogeneous Knight shift [6], which lifts the degeneracy of the nuclear Zeeman energy for different nuclei and prevents the spin flip-flop; on the other hand, electron-mediated nuclear spin flip-flop enhances the nuclear spin diffusion and the enhancement decreases from the center to the edge of the dot.

Our numerical simulation shows that whether one mechanism dominates the other is largely determined by the external magnetic field B_0 . Figures 1 and 2 show the diffusion coefficient $D(x, y)$ under $B_0 = 0.2 \text{ T}$ and $B_0 = 2 \text{ T}$. We can see that under a small magnetic field, the electron-mediated flip-flop greatly enhances the nuclear spin diffusion near the center of the

⁴ The hyperfine coupling rate A_i , although inhomogeneous over a larger scale, only changes slightly from one nuclear spin to its nearby spins, so in summation over the nearby lattice sites, we still have an approximate lattice symmetry for the jump rate W_{ik} .

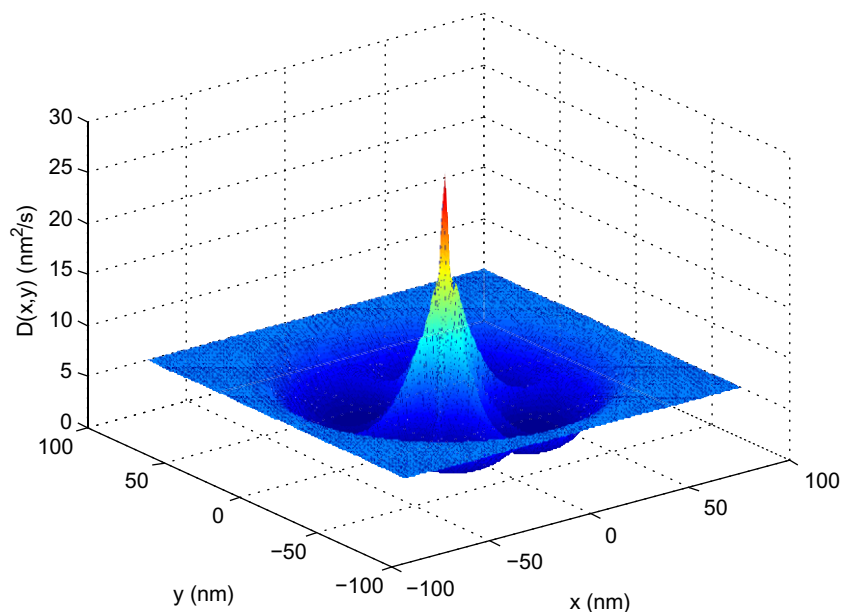


Figure 1. The diffusion coefficient $D(x, y)$ under $B_0 = 0.2$ T. The narrow high peak at the center of the dot is due to electron-mediated nuclear spin flip-flop, and the wide dip is due to inhomogeneous Knight shift.

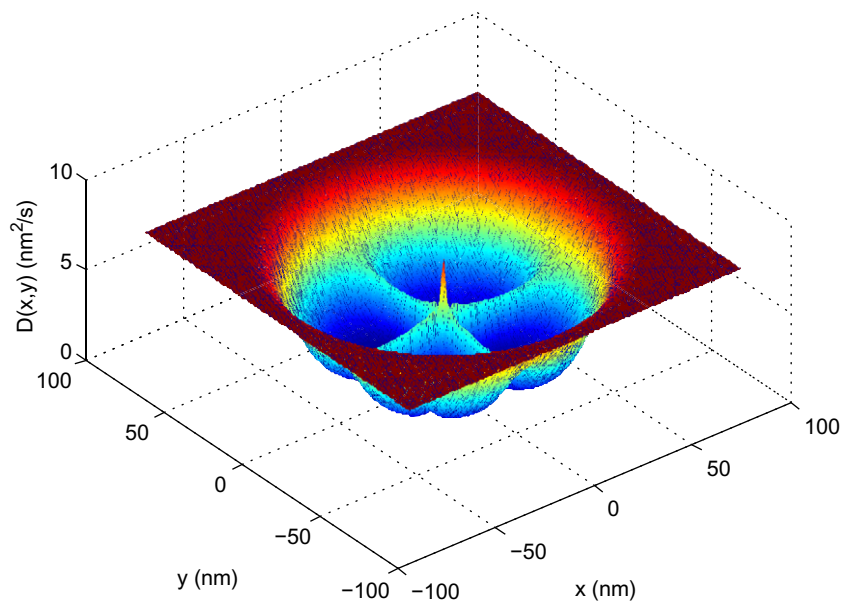


Figure 2. The diffusion coefficient $D(x, y)$ under $B_0 = 2$ T. The inhomogeneous Knight shift dominates in this case, so diffusion is generally suppressed within the Fock–Darwin radius.

dot, causing a sharp peak in $D(x, y)$. In a large magnetic field, however, such enhancement is negligible compared to the Knight shift, which suppresses the nuclear spin diffusion, yielding a wide dip in $D(x, y)$. The dependence on the strength of the magnetic field can be easily explained with the effective Hamiltonian (equations (10)–(12)): the electron-mediated flip-flop

term is inversely proportional to B_0 , whereas the Knight shift term is independent of B_0 . We note that the reason why we have a narrower peak than the dip is because the Knight shift term is proportional to the hyperfine coupling rate (Gaussian distribution in the x - y plane), whereas the electron-mediated flip-flop term is proportional to the product of two nuclei's hyperfine coupling rates. We also note that the 2D diffusion coefficient $D(x, y)$ in figures 1 and 2 does not have azimuthal symmetry because in our calculation we assume that the nuclear spins are in a square lattice with no azimuthal symmetry.

3. Comparison with experiments

To compare with experiments, we numerically solve the diffusion equation (equation (25)) under certain initial and boundary conditions. For the initial condition, since the nuclear spins are partially polarized through the DNP process from the hyperfine interaction with the electron spin [13]–[16], it is reasonable to expect that right after the DNP process, the polarization distribution $\langle I_k^z \rangle$ is proportional to the hyperfine interaction rate. So, in the following calculation, we assume $\langle I_k^z \rangle \propto A_k \propto \exp[-(x_i^2 + y_i^2)/l_0^2]$ at $t = 0$ for solving the diffusion equation (25). For the boundary condition, we can assume naturally that $\langle I_k^z \rangle$ approaches zero when the radius goes to infinity. However, in numerical calculation, we have to take a finite radius. To make the spin diffusion possible, this finite radius has to be significantly larger than the radius of the size l_0 of the initial electron wave packet. In the calculation, we take a radius of about 300 nm (10 times l_0) so that the total number of nuclear spins inside is about 100 times the number of initially partially polarized nuclear spins within the electron's wave packet. With such a choice, we expect the cutoff error to be at the per cent level.

First, to compare with the experiments in [18], we calculate the relaxation of the Overhauser field $h^z(t) = \sum_k A_k \langle I_k^z(t) \rangle$ under different electron states and different values of the external magnetic field B_0 , and show the results in figure 3. We note that for the double quantum dot system in [18], if the electron stays in the (2, 0) singlet state, the electron spin has $S_z \equiv 0$; therefore, it basically has no influence on the nuclear spin diffusion. In this case, the nuclear spin diffusion is merely governed by intrinsic nuclear dipole–dipole interaction. However, for the electron in the (1, 1) state, with the magnetic field in the range of tens of mT as in this experiment, the electron-mediated spin diffusion dominates the Knight shift and accelerates the nuclear spin relaxation. That is why one can see two effects from figure 3: (i) electrons in the (1, 1) state will speed up the decay of the Overhauser field compared to electrons in the (2, 0) state; (ii) a smaller magnetic field gives a faster decay of the Overhauser field. Both these effects agree well with the experimental observations in [18]. The decay time is also consistent in terms of the order of magnitude.

With a much larger magnetic field (say, $B_0 = 2$ T, as in experiments in [19]), the electron-mediated nuclear spin diffusion is suppressed, and the Knight shift plays a more important role. The Knight shift suppresses the nuclear spin diffusion, yielding a relaxation time of the Overhauser field that is significantly larger than that in bulk material. Figure 4 shows the decay of the Overhauser field in this case, and we can fit the curve with an effective constant diffusion coefficient at about $D_{\text{eff}} \approx 0.7 \text{ nm}^2 \text{ s}^{-1}$. Compared with the diffusion coefficient in the bulk material ($D \approx 7 \text{ nm}^2 \text{ s}^{-1}$), a suppression factor of 10 is obtained by applying a strong magnetic field. The experiments performed in [19] measured an effective diffusion coefficient 50 times smaller than the value in the bulk system. The other suppression effect of nuclear spin diffusion involved in [19] comes from the inhomogeneous quadruple shift of nuclear spin

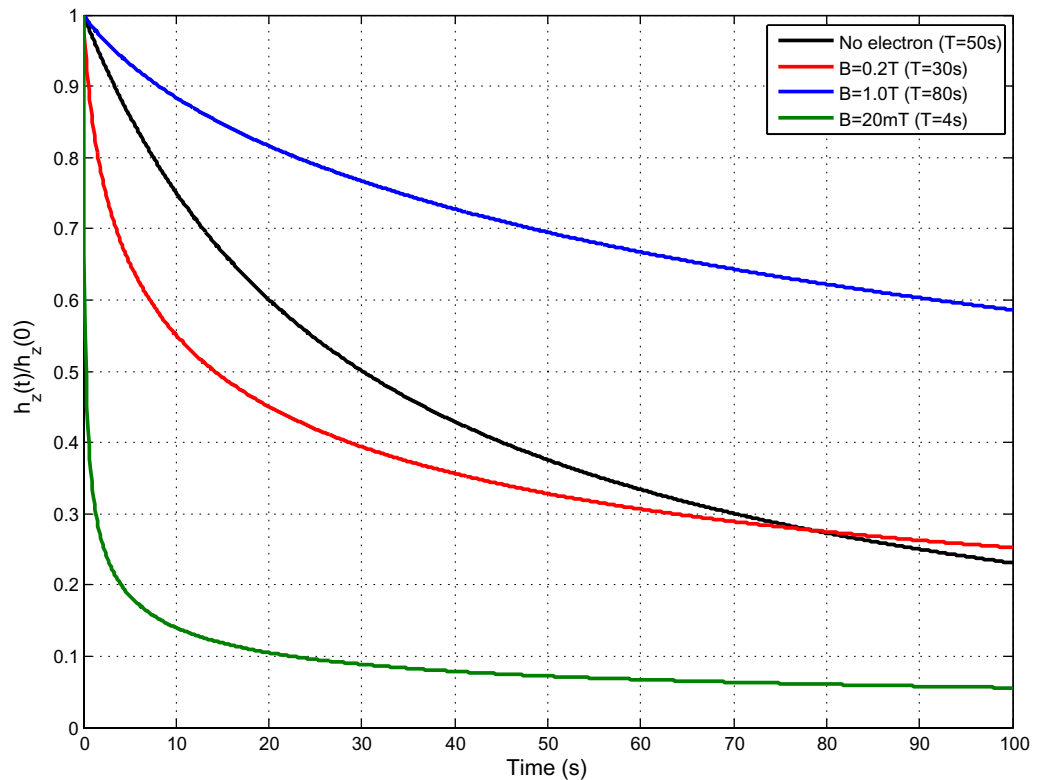


Figure 3. Decay of the Overhauser field under various small magnetic fields. The solid line refers to the case where the electron stays in the $(2, 0)$ singlet state and has no role in nuclear spin diffusion.

energy [22, 29]. Similar to the inhomogeneous Knight shift, the inhomogeneous quadruple shift can also make the nuclear spin flip-flop process off-resonant and therefore suppressed. The quadruple shift in those InGaAs quantum dot systems can have a much stronger influence on the energy spectrum of the nuclear Hamiltonian when compared with the Knight shift. Therefore, an intense suppression of nuclear spin diffusion can be induced by quadruple shift, and Overhauser field relaxation time up to 1 h was seen in [22].

The experiment in [20] studies relaxation of the Overhauser field under different pumping times for the DNP process. With a shorter DNP pumping time, the nuclear spin polarization may have a narrower distribution in space [17]. Although we do not know the exact distribution profile of the nuclear spin polarization from a short DNP pump process, we can assume that the distribution of $\langle I_k^z \rangle$ is still simply a Gaussian but with radius $r_0 < l_0$, to model the experiment qualitatively. Taking this $\langle I_k^z \rangle$ as the initial condition, we can calculate relaxation of the corresponding Overhauser field from the same diffusion equation (25), and the result is shown in figure 5. The result indicates that a narrower distribution of initial nuclear spin polarization leads to a faster decay of the Overhauser field, which is consistent with the experimental result in [17]. This effect can be explained by noting that diffusion is much stronger near the center of the dot due to the electron-mediated diffusion peak (see figure 1), so a shorter relaxation time is obtained if the initial polarization is more concentrated near the dot center.

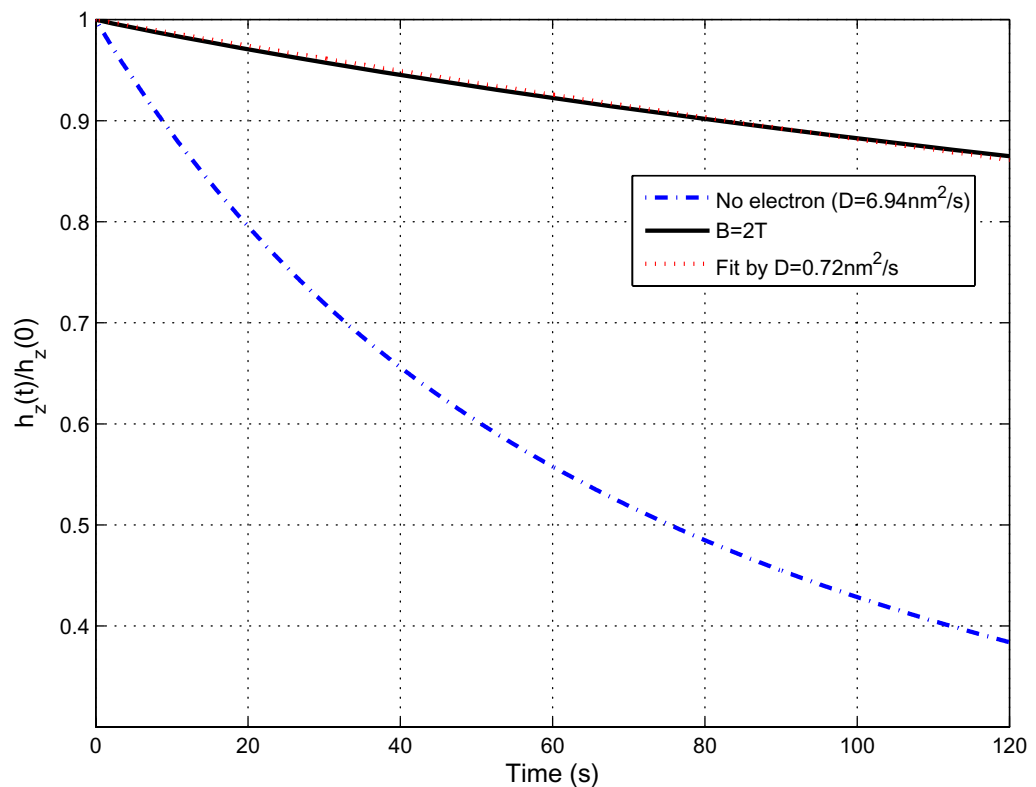


Figure 4. Decay of the Overhauser field under a strong magnetic field. The solid line shows the dynamics of the Overhauser field under $B = 2$ T and the dotted line is a fit performed using a constant diffusion coefficient.

4. Summary and discussion

In summary, we established an effective method for calculating the long time dynamics of the Overhauser field under nuclear spin diffusion and showed that the confined electron in a quantum dot can both enhance the decay of the Overhauser field by mediating nuclear spin flip-flop and suppress the decay via inhomogeneous Knight shift. Which effect dominates the other depends critically on the magnitude of the external magnetic field. With this method, we numerically simulated the relaxation process of the Overhauser field under different electron spin configurations, external magnetic field and initial nuclear spin polarization distribution. The results agree reasonably well with a series of recent experimental observations.

In our calculation, we ignored the quadruple shifts of nuclear spins, which are nonexistent in certain systems such as ^{13}C -nanotube quantum dots [30], negligible in strain-free semiconductor nanostructures such as epitaxially grown droplet quantum dots [31] and dominated by Zeeman energy under a magnetic field B_0 much larger than the equivalent quadruple magnetic field B_Q (of the order of 0.1 T for InAs quantum dots as in [22]). For quantum dots with strong inhomogeneous strain-induced quadruple shifts, we believe that nuclear spin diffusion will be further suppressed by them in a similar way as by the inhomogeneous Knight shift. Details of the influence of quadruple shifts on nuclear spin dynamics can be found in [32] and are beyond the scope of this paper. We also note that considering more than one species of nuclei

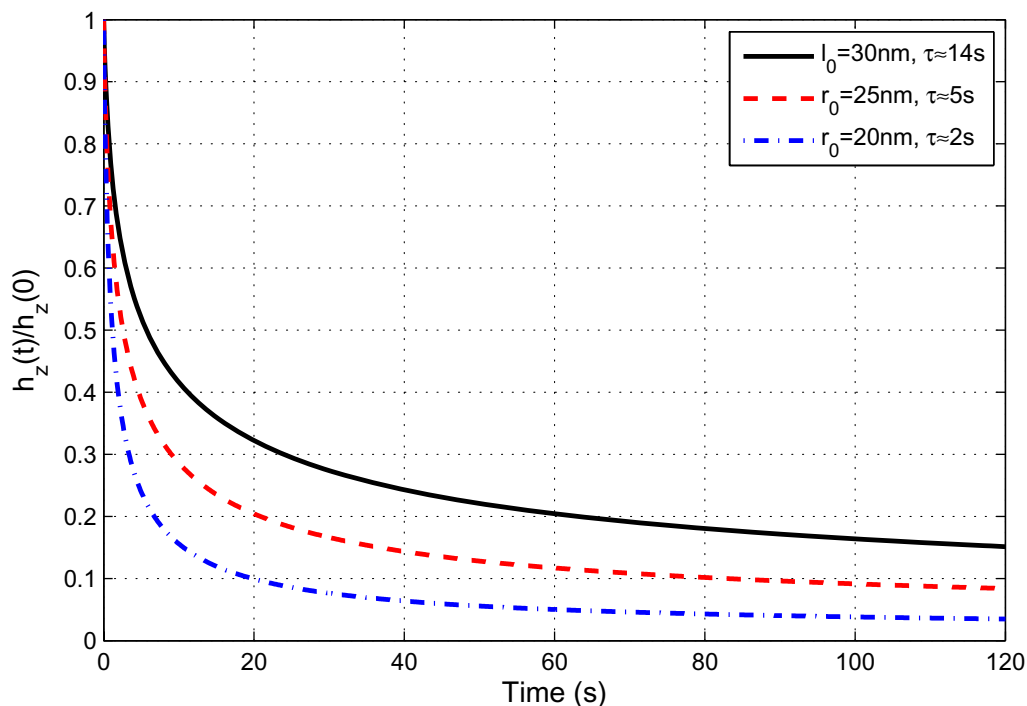


Figure 5. Overhauser decay of the Overhauser field under various initial distributions of the nuclear polarization. The solid line refers to the case with a long DNP pump time that gives a Gaussian distribution with the size characterized by the Fock–Darwin radius l_0 . Other lines correspond to a narrower polarization distribution characterized by a Gaussian with size $r_0 < l_0$.

in the diffusion process, as in real experiments, should give a moderate increase of the diffusion coefficient because more nuclear spin flip-flop channels (including those between two different species of nuclei) will be involved, but is unlikely to alter the electron’s role in nuclear spin diffusion we discussed above.

Our results inform researchers of ways of maintaining the DNP-generated Overhauser field as long as possible. Firstly, one can apply a large magnetic field to effectively suppress the electron-mediated nuclear spin diffusion. Secondly, one can choose a quantum dot system with a large inhomogeneous Knight shift or quadruple shift to suppress the intrinsic nuclear dipole–dipole spin diffusion. These methods together can give us a rather long relaxation time of the Overhauser field.

In this paper, we have focused on the time dynamics of the **expectation value** of the Overhauser field, since this is the quantity that has been measured in several recent experiments. Similar methods could be applied to calculate the dynamics of the **variance** of the Overhauser field, and in terms of time scale, they should be more or less the same. We also want to point out here that during the DNP process, nuclear spin diffusion also takes place. The final distribution of the nuclear spin polarization and its variance may depend on the balance between the DNP pump rate and the nuclear spin diffusion rate ([13]–[16], [18]). To understand this balance, a detailed knowledge of the specific DNP process will be required. We believe that our analysis and calculation method that fully incorporates the electron’s role in nuclear spin diffusion can

help achieve such an understanding and possibly further suppress the fluctuation of nuclear spins.

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