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Effect of nuclear polarization on spin dynamics in a double quantum dot

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We study spin dynamics and singlet-triplet decoherence due to the hyperfine interaction in a parabolic double quantum dot, focusing on the effect of nuclear-spin polarization on the time evolution of the singlet probability. The probabilities for the singlet state exhibit damped oscillations, which do not change considerably when the nuclear-spin polarization is small. We derive expressions for the mean and variance of the saturation value of the singlet probability in cases where the hyperfine field has a nonzero mean. We demonstrate that the polarization could be deduced from experiments by measuring both the mean and variance of the asymptotic singlet probability.

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I. INTRODUCTION

In a quantum-mechanical system, the interaction with the environment causes decoherence. In order to develop quantum devices, the problems related to decoherence must be solved in some way. A setup of electrons confined in quantum dots has emerged during recent years as one of the most interesting alternatives for quantum computing architecture. In low temperatures, the most significant decoherence source is the hyperfine interaction of the electrons with the surrounding nuclear spins. There are several methods to suppress the decoherence induced by the hyperfine field. The narrowing of the hyperfine field distribution is one method. This is realized, e.g., by gate-controlled Rabi oscillations or by optical preparation of nuclear spins. The polarization of the nuclear spins could also diminish the decoherence rate, but nearly 100% polarization is not feasible. However, the decoherence rate may be substantially increased by a nuclear-spin pumping cycle, which suppresses the hyperfine field fluctuation by a factor of 70. Thus it is very important to know the effect of the shape of the hyperfine field distribution on the decoherence of the spin system.

In the following, we analyze the singlet-triplet decoherence in a double quantum dot. This phenomenon has recently been measured by Laird et al. They controlled the system parameters by varying the gate voltage over the system, which affected the exchange energy. The singlet probability was observed to saturate to a value which depends only on the ratio of the hyperfine field strength and the exchange energy. This is in accordance with the model developed by Coish and Loss, where they describe the system using a $2 \times 2$ Hamiltonian matrix. We evaluate numerically the singlet probability as a function of time, concentrating on the changes the nuclear-spin polarization has on the dynamics. In addition, we derive expressions for the asymptotic singlet probability and its variance in a situation where the average of the hyperfine field differs from zero.

II. SPIN DYNAMICS

A. Model

We investigate a system of two electrons confined in a double quantum dot. The hyperfine interaction between electrons and nuclei is approximated through a random mean hyperfine field $\mathbf{h}$. The Hamiltonian of the system reads

$$ H = \epsilon S_z + h_1 \cdot S_1 + h_2 \cdot S_2 - J \sum_{i=1}^{2} S_i \cdot S_i, $$

where $S_i$ are the spin operators of the electrons, $h_i$ are the hyperfine fields the electrons interact with, $\epsilon$ is the Zeeman energy, and $J$ is the exchange energy. We write the Hamiltonian in a more compact form

$$ H = \epsilon S_z + \mathbf{h} \cdot \mathbf{S} + \delta \mathbf{S} \cdot \delta \mathbf{S} + \frac{J}{2} \mathbf{S} \cdot \mathbf{S} - J, $$

where $\mathbf{h} = h_1 \mathbf{h}_1 + h_2 \mathbf{h}_2$, $\mathbf{S} = S_1 + S_2$, $\delta \mathbf{h} = h_1 - h_2$, and $\delta \mathbf{S} = S_1 - S_2$. If the external magnetic field is large compared to the hyperfine field, the coupling of the triplet states having $S_z = \pm 1$ with the states having $S_z = 0$ is weak due to the Zeeman splitting. This is the case in recent experiments of spin dynamics in two-electron double quantum dots as our numerical simulations using realistic parameters from these experiments show that the two triplet states with $S_z = \pm 1$ remain unoccupied. The relative error of the singlet probability caused by the exclusion of the states with $S_z = \pm 1$ is under 0.001. Hence, we may restrict our analysis to the dynamics of the singlet state $|S\rangle$ and triplet state $|T_0\rangle$. The reduced Hamiltonian (details of the calculation are given in Ref. 16) is now

$$ H = \frac{J}{2} \mathbf{S} \cdot \mathbf{S} + \delta \mathbf{h} \cdot \delta \mathbf{S}, $$

which in matrix form reads

$$ H = \begin{pmatrix} 0 & \delta h \\ \delta h^T & J \end{pmatrix}. $$

The exact time dependence of the wave function can be calculated from the relation $\phi(t) = \exp(-iHt/\hbar)\phi(0)$. We denote $\phi(t) = (\alpha(t)\beta(t))^T$ and use the initial condition $\phi(0) = (10)^T$. We obtain the coefficient $\alpha(t)$ from the relation,
study the effect of the polarization. We therefore resort to numerical evaluation of the integral. Next, we will calculate the integral, which is not easy to calculate analytically, and we will assume that it can be approximated by the average over a finite number of realizations. Hence, we approximate the polarization by the averaging over finite number of realizations. Hence, over the statistical ensemble of hyperfine spins, we assume that the singlet probability oscillates sinusoidally. In order to obtain the average over the statistical ensemble of hyperfine spins, we assume that the couplings and variances are normally distributed with mean and variance and . The ensemble average of the singlet probability as a function of time over the hyperfine field is given by

\[
\langle P_S(t) \rangle = \frac{1}{\sqrt{2\pi\sigma_0^2}} \int_{-\infty}^{\infty} \exp\left(-\frac{(\Delta h - h_0)^2}{2\sigma_0^2}\right) P_S(t) \, d(\Delta h),
\]

This integral is not easy to calculate analytically, and we resort to numerical evaluation of the integral. Next, we will study the effect of the polarization and variance on the singlet probability \(\langle P_S(t) \rangle\).

\[
\alpha(t) = \psi(0)^T A \begin{pmatrix} \exp(i\lambda_{1,2}t) & 0 \\ 0 & \exp(i\lambda_{3,2}t) \end{pmatrix} A^{-1} \psi(0),
\]

where \(\lambda_{1,2} = \frac{i}{2}(J \pm \sqrt{4(D\delta h^2 + J^2)})\) are the eigenvalues of \(H\) and \(A\) is the orthonormal matrix composed of the eigenvectors of \(H\). The singlet probability, given by \(|\alpha(t)|^2\), is now

\[
P_S(t) = \frac{1}{2} \left[ 1 + \frac{J^2}{D^2} + \left(1 - \frac{J^2}{D^2}\right) \cos(Dt) \right],
\]

where \(D = \sqrt{4(D\delta h^2 + J^2)}\). For constant \(\delta h\), the singlet probability oscillates sinusoidally. We observe that the curves are close to each other when the ratio of the mean and standard deviation \(h_0/\sigma_0 > 2\). For the curves with largest \(h_0\), the ratio is over 2 and these curves have notably larger amplitude. These results indicate that one may estimate the polarization of the hyperfine field by using the amplitude of the singlet probability measurements. We estimated that the fluctuation of the measurements of Ref. 15 corresponds to around 50 realizations. The increase in the amplitude due to the polarization could be observed only when it exceeds the variation in the amplitude caused by the averaging over finite number of realizations. Hence, only for \(h_0/\sigma_0 > 2\) one might have such a large oscillations that could be used for more precise determination of the polarization. Reilly et al.\(^{14}\) could suppress the fluctuations of the hyperfine field component parallel to the external magnetic field in their experiment by a factor of 70. Also the polarization increased slightly, so that the ratio \(h_0/\sigma_0\) increased by 2 orders of magnitude. This results in a very slowly damping oscillation for the singlet probability near \(P_S = 1\). Using this suppression method, it would be possible to measure the singlet oscillations more accurately using the scheme of Laird et al.,\(^{15}\) as the period of the oscillations is longer and fluctuations smaller, and analyze the polarization of the hyperfine field.

C. Spin saturation

Although it is not trivial to represent the average of \(P_S(t)\) over the hyperfine field distribution in a simple analytic form, the averaging is easy to calculate for the saturation value of \(P_S\). We define the time average of the singlet probability \(\bar{P}_S = \frac{1}{T} \int_0^T P_S(t) \, dt\). When the upper limit of the time average is

<table>
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<th>(P_S)</th>
<th>(h_0/J)</th>
<th>(\sigma_0/J)</th>
<th>Color (gray scale)</th>
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<tr>
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Figures 1(a)–1(c) represent the time-dependent singlet probability \(\langle P_S(t) \rangle\) for different asymptotic singlet probabilities: (a) \(\langle P_S(\infty) \rangle = 0.82\), (b) 0.91, and (c) 0.95, corresponding to measurements of singlet probabilities with exchange energies \(J = 25, 42,\) and \(60\) neV shown in Fig. 4 of Ref. 15. We denote that the ensemble averaging of the sinusoidal oscillation results to damping of the singlet oscillation. The values of the mean \(h_0\) and standard deviation \(\sigma_0\) used in each figure (shown in the Table I) all give the same asymptotic singlet probability. We observe that the curves are close to each other when the ratio of the mean and standard deviation \(h_0/\sigma_0 < 2\). For the curves with largest \(h_0\), the ratio is over 2 and these curves have notably larger amplitude. These results indicate that one may estimate the polarization of the hyperfine field by using the amplitude of the singlet probability measurements. We estimated that the fluctuation of the measurements of Ref. 15 corresponds to around 50 realizations. The increase

![Graphs showing singlet probability over time](image-url)
eraging $T$ is large, the oscillatory term in the singlet probability given by Eq. (6) is small, as the oscillations decay with increasing time. Then we obtain the saturation value from the time-independent part of Eq. (6),

$$\bar{P}_S = \frac{1}{2} \left( 1 + \frac{J^2}{D^2} \right).$$

(7)

Next, we calculate the asymptotic singlet probability $\langle \bar{P}_S \rangle$, which is an average of the saturation value $\bar{P}_S$ over the hyperfine field realizations,

$$\langle \bar{P}_S \rangle = \frac{1}{\sqrt{2\pi} \sigma_0} \int_{-\infty}^{\infty} \exp \left( -\frac{(\delta h - h_0)^2}{2\sigma_0^2} \right) \bar{P}_S,$$

which leads to the formula for the mean of the asymptotic singlet probability,

$$\langle \bar{P}_S \rangle = \frac{1}{2} + \sqrt{\frac{\pi}{2}} \frac{J}{4 \sigma_0} \exp \left( \frac{J^2}{8 \sigma_0^2} \right)$$

\times \operatorname{Re} \left[ \exp \left( \frac{iJh_0}{2\sigma_0} \right) \operatorname{erfc} \left( \frac{J + 2iJh_0}{2\sqrt{2\sigma_0} \sigma_0} \right) \right].$$

(9)

This result is in agreement with the expression derived by Klauser et al.,\textsuperscript{11} when the Rabi oscillations of the exchange energy vanish. In the case $h_0=0$, we have

$$\langle \bar{P}_S \rangle = \frac{1}{2} + \sqrt{\frac{\pi}{2}} \frac{J}{4 \sigma_0} \exp \left( \frac{J^2}{8 \sigma_0^2} \right) \operatorname{erfc} \left( \frac{J}{2\sqrt{2\sigma_0}} \right).$$

(10)

When the standard deviation $\sigma_0$ approaches zero, the normal distribution in the integrand of Eq. (8) may be approximated by a delta function. Then the average is obtained from the Eq. (7) by substitution $\delta h \approx h_0$ and we have

$$\langle \bar{P}_S \rangle = \frac{1}{2} \left( 1 + \frac{1}{4} \right).$$

(11)

The exchange energy $J$ gives the relevant energy scale of the system. Thus, it is natural to measure $h_0$ and $\sigma_0$ in units of $J$.

In Fig. 2, the asymptotic triplet probability $\langle \bar{P}_T \rangle = 1 - \langle \bar{P}_S \rangle$ as a function of the mean of the hyperfine field is shown for several values of the standard deviation of the hyperfine field. For small standard deviation, the distribution of $\delta h$ is concentrated around the mean. When the mean is increased, most of the hyperfine field values are positive and the decoherence is stronger. Hence, the asymptotic value $\langle \bar{P}_T \rangle$ approaches $\frac{1}{2}$. For larger values of the hyperfine field standard deviation, the hyperfine field has a large portion of negative values even in the cases where the mean is far from zero. Therefore, in the case $\frac{\sigma_0}{J}=2.0$ the asymptotic value does not change considerably when the mean increases.

In Fig. 3, $\langle \bar{P}_T \rangle$ is shown as a function of the standard deviation for different values of the mean of the hyperfine field. For zero standard deviation, $\langle \bar{P}_T \rangle$ is given by Eq. (11). In the case of nonzero mean, the triplet probability has a finite value at $\sigma_0=0$. All values of the hyperfine field are then positive. When the standard deviation is increased keeping
In the case $r_0 = 0$, hence, it might be difficult to determine $r_0$ experimentally because the accuracy of the asymptotic variance measurement should be high.

**III. SUMMARY**

In summary, we have analyzed the singlet-triplet decoherence in a double quantum dot using model based on a $2 \times 2$ Hamiltonian matrix. We evaluated numerically the time dependence of the singlet probability for several hyperfine field distributions. We observed that a small nonzero mean on the hyperfine field does not have a considerable effect on the singlet oscillations. We calculated exact formulas for the asymptotic singlet probability and its variance for the case of Gaussian hyperfine field distribution. The asymptotic triplet probability was shown to have a minimum when variance is close to the mean. We also demonstrated the possibility to measure the ratio of the mean and standard deviation of the hyperfine field by measuring the asymptotic mean and variance of the singlet probability.

**ACKNOWLEDGMENTS**

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**APPENDIX: VARIANCE OF THE ASYMPTOTIC SINGLET PROBABILITY**

For the time average of the squared singlet probability $\bar{P}_S^2 = \frac{1}{T} \int_0^T \bar{P}_S(t)^2 dt$, we have

$$\bar{P}_S^2 = \frac{1}{8} \left( 3 + 2 \frac{J^2}{D^2} + 3 \frac{J^4}{D^4} \right).$$

From this, one can calculate the ensemble average $\langle \bar{P}_S^2 \rangle$, and using this, we obtain the variance of the asymptotic singlet probability $\sigma^2(\bar{P}_S) = \langle \bar{P}_S^2 \rangle - \langle \bar{P}_S \rangle^2$.

$$\sigma^2(\bar{P}_S) = \frac{1}{64} \left( 8 + \frac{J^2}{\sigma_0^2} - \sqrt{2\pi} \exp \left( \frac{J^2 - 4\hbar_0^2}{8\sigma_0^2} \right) \Re \left[ \exp \left( \frac{i\hbar_0}{2\sigma_0^2} \right) \text{erfc} \left( \frac{J + 2i\hbar_0}{2\sqrt{2}\sigma_0} \right) \right] + \sqrt{2\pi} \frac{J^2}{\sigma_0^2} \exp \left( \frac{J^2 - 4\hbar_0^2}{8\sigma_0^2} \right) \right).$$

When the mean is zero, this formula simplifies to the expression,

$$\sigma^2(\bar{P}_S) = \frac{1}{64} \left( 8 - \sqrt{2\pi} \frac{3J^2}{4\sigma_0^2} + \frac{J}{\sigma_0^2} \exp \left( \frac{J^2}{8\sigma_0^2} \right) \text{erfc} \left( \frac{J}{2\sqrt{2}\sigma_0} \right) + \frac{J^2}{\sigma_0^2} \right).$$

In the case $\sigma_0 = 0$, we obtain the following formula:

$$\sigma^2(\bar{P}_S) = \frac{1}{8} \left( 1 - \frac{2}{4\left( \frac{\hbar_0}{J} \right)^2} + \frac{1}{4 \left( \frac{\hbar_0}{J} \right)^2} \right).$$