Hyperfine interaction induced decoherence of electron spins in quantum dots

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(Received 13 July 2006; revised manuscript received 11 September 2006; published 14 November 2006)

We investigate in detail, using both analytical and numerical tools, the decoherence of electron spins in quantum dots (QDs) coupled to a bath of nuclear spins in magnetic fields or with various initial bath polarizations, focusing on the longitudinal relaxation in low and moderate field and polarization regimes. An increase of the initial polarization of nuclear-spin bath has the same effect on the decoherence process as an increase of the external magnetic field, namely, the decoherence dynamics changes from smooth decay to damped oscillations. This change can be observed experimentally for a single QD and for a double-QD setup. Our results indicate that substantial increase of the decoherence time requires very large bath polarizations, and the use of other methods (dynamical decoupling or control of the nuclear spins distribution) may be more practical for suppressing decoherence of QD-based qubits.

DOI: 10.1103/PhysRevB.74.205313 PACS number(s): 75.10.Jm, 03.65.Yz, 03.67.−a, 02.60.Cb

I. INTRODUCTION

Quantum dots (QDs) are very promising candidates for future implementation of quantum computations: an electron spin in a QD is a natural two-state quantum system, which can be efficiently manipulated by the external magnetic fields and gate voltages.[1,2] Also, the QD-based architectures are potentially scalable, and rely on well-developed semiconductor technology.[3] However, due to interaction with the environment, the electron spin loses coherence very quickly, on a time scale of order of nanoseconds for typical GaAs QDs.[1] It is vitally important for realization of QD-based quantum computing to understand the decoherence dynamics in detail, in order to find practical ways of decoherence suppression. Moreover, decoherence of open systems is of fundamental interest for understanding of the quantum phenomena taking place in mesoscopic systems,[4–6] and therefore attracts much attention from scientists working in the areas of nanoscience, spintronics, and quantum control.

Among different sources of decoherence relevant for an electron spin in a QD, the decoherence by the bath of nuclear spins (spin bath) is dominant for magnetic fields less than a few T, and experimentally relevant temperatures of tens or hundreds of mK. Much research has been focused on the case of a large external magnetic field or large bath polarizations, where the perturbation theory allows an extensive analysis.[7–10] But the interesting and experimentally relevant regime of moderate magnetic fields and/or moderate bath polarization has received much less attention.

Below, we study in detail the influence of moderate magnetic fields and bath polarization on the longitudinal decoherence of a single spin in a quantum dot, and two spins located in neighboring QDs, where the perturbation theory is not applicable. In this regime, as the magnetic field or the bath polarization increase, the dynamics of the electron spins undergoes a transition from simple overdamped decay to underdamped oscillations, and these oscillations can be detected using existing experimental schemes. In this transition, the increase of bath polarization affects the decoherence dynamics in exactly the same manner as the increase of the magnetic field. Our results also show that suppression of decoherence requires very large bath polarizations, suggesting that the use of such methods as dynamical decoupling,[1,11,12] or control of the nuclear spins distribution,[13] may be more practical.

Theoretical description of the spin-bath decoherence is a very complex problem,[14] where strong correlation and essentially non-Markovian bath dynamics play an important role.[7,15,16] In contrast with the well studied boson-bath decoherence,[4,6] decoherence by a spin bath has not yet been understood in detail, especially in moderate external magnetic fields.

II. SINGLE ELECTRON SPIN IN A QD

An electron spin in a QD interacting with a bath of nuclear spins is described by the Hamiltonian which includes the Zeeman energy of the electron spin in the external magnetic field B_0 and the contact hyperfine coupling:[17,18] $\mathcal{H}=H_0 S_z+\sum_{k=1}^{N} A_k \mathbf{S}\cdot\mathbf{I}_k$, where $\mathbf{S}$ is the operator of the electron spin, $\mathbf{I}_k$ is the operator of the kth bath spin $(k=1,2,\ldots,N)$, and $A_k=(8\pi/3)g_e^{*}\mu_B g_n \mu_n u(\mathbf{x}_k)$ is the contact hyperfine coupling which is determined by the electron density $u(\mathbf{x}_k)$ at the site $\mathbf{x}_k$ of the kth nuclear spin and by the Landé factors of the electron g_e^{*} and of the nuclei g_n. The terms omitted in the above Hamiltonian, such as the Zeeman energy of the nuclear spins, the anisotropic part of the hyperfine coupling, etc., are small, and can be safely neglected at the nanosecond time scale, which is considered here.

In spite of the apparent simplicity of the Hamiltonian, it is very difficult to determine the dynamics of the central spin $\mathbf{S}(t)$. Previously, the quasistatic approximation (QSA) for the nuclear-spin bath, which treats $\sum_k A_k \mathbf{I}_k$ as a constant, has often been invoked.[19–22] Analytical calculations beyond the QSA have been carried out only for large magnetic field and/or large bath polarizations,[7–10] where the perturbative approach is valid. Although many qualitative arguments support QSA, its validity has not yet been checked in detail.

Below, along with explicit analytical solutions, we provide direct verification of our analytics by employing the exact numerical simulations for medium-size ($N=20$) baths, and approximate simulations for large ($N=2000$) baths. The agreement between all three methods ensures us that our findings do not depend on the approximations involved.

The analytical calculations within the QSA can be performed in different ways which all give the same results. The conceptually simplest way is to assume a uniform electron density in the QD, so that all A_k are the same, $A_k=A$, and the Hamiltonian can be written as $\mathcal{H}=H_0S_z+A\mathbf{S}\cdot\mathbf{I}$, where $\mathbf{I}=\Sigma_k\mathbf{I}_k$ is the total nuclear spin of the bath. This Hamiltonian can be analyzed exactly, since $\mathbf{I}^2$ and I_z+S_z are the integrals of motion.

First, we consider an unpolarized bath, with the density matrix $\rho_b(0)=(1/2^N)\mathbf{1}_1\otimes\cdots\otimes\mathbf{1}_N$, where $\mathbf{1}_k$ is the unity matrix for kth bath spin. This density matrix can be rewritten in the eigenbasis of $\mathbf{I}^2$, I_z as $\rho_b(0)=\Sigma_{I=0}^{N/2}\Sigma_{M=-I}^{I}P(I,M)|I,M\rangle\langle I,M|$ where $M=I_z$. Assuming that the initial state of the electron is $|\uparrow\rangle$, the quantum-mechanical average of the z component of the electron spin at time t is

$$\sigma_z(t)\equiv 2\langle S_z(t)\rangle=\sum_{I,M}P(I,M)\frac{B^2+C^2\cos\Omega t}{\Omega^2}, \qquad (1)$$

where $C=A\sqrt{(I-M)(I+M+1)}$, $B=H_0+A(M+1/2)$, and $\Omega^2=B^2+C^2$. Due to the symmetry of the problem and the initial condition, $\sigma_x(t)=\sigma_y(t)=0$, so we omit these components. The distribution function $P(I,M)$ can be calculated[23] and for large N and I it is approximated by a Gaussian distribution $P(I,M)\approx(I/D\sqrt{2\pi D})e^{-I^2/2D}$ where $D=N/4$. Replacing the summation by integration in Eq. (1), we find

$$\sigma_z(t)=1-2W(\lambda,D;t), \qquad (2)$$

and the function $W(\lambda,D;t)$ has the form

$$W=\frac{D}{\lambda^2}-\frac{D}{\lambda^2}e^{-Dt^2/2}\cos\lambda t+i\sqrt{\frac{\pi}{2}}\frac{D^{3/2}}{2\lambda^3}e^{-\lambda^2/2D}\times\left[\Phi\left(\frac{Dt-i\lambda}{\sqrt{2D}}\right)-\Phi\left(\frac{Dt+i\lambda}{\sqrt{2D}}\right)+2\Phi\left(\frac{i\lambda}{\sqrt{2D}}\right)\right], \qquad (3)$$

where $\Phi(x)$ is the error function. In this equation, we took $A=1$, and introduced the notation $\lambda=H_0/A$; this corresponds to normalized energy and time scales, so that the time t is measured in the units of $1/A$. The dynamics of $\sigma_z(t)$ for several values of λ are shown in Figs. 1 and 2.

Before discussing the above results, we consider next a polarized bath, assuming that its initial state is described by a density matrix $\rho_b(0)=(1/Z_\beta)\exp(-\beta M)$, where β is the inverse spin temperature, and $Z_\beta=[2\cosh(\beta/2)]^N$ is the statistical sum, and the initial bath polarization is $p\equiv\langle M\rangle/(N/2)=-\tanh(\beta/2)$. For large spin temperatures, the polarization is small, $p\approx-\beta/2$, and we approximate $P(I,M)\approx(I/D\sqrt{2\pi D})e^{-D\beta^2/2}e^{-I^2/2D}e^{-\beta M}$, so that

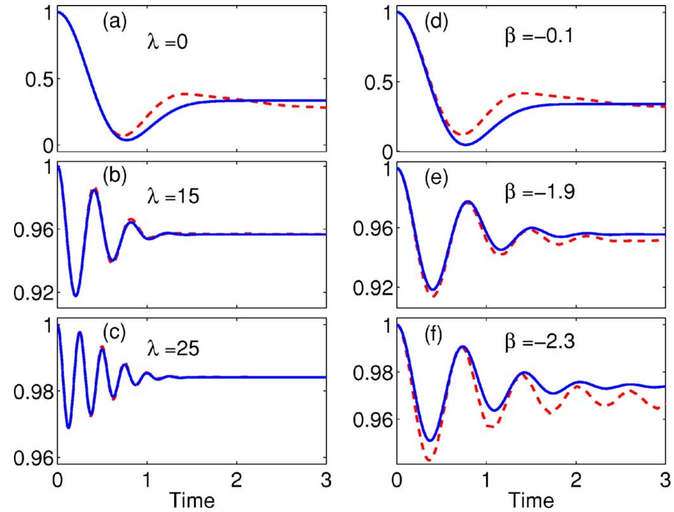

FIG. 1. (Color online) Electron-spin decoherence in various magnetic fields [(a)–(c)] and with polarized initial nuclear spin baths [(d)–(f)] for $N=20$. The red dashed curves denote the exact numerical simulations results for $N=20$, and the blue solid curves correspond to the analytical results. The numerical results agree well with the analytical predictions, and the underdamped oscillations appear once λ or κ is larger than $\sqrt{N}$.

$$\sigma_z(t)=1-2W(\kappa,D;t), \qquad (4)$$

where $\kappa=D\beta$, and the function $W(\kappa,D;t)$ is defined by Eq. (3). The dynamics of $\sigma_z(t)$ for several values of β is shown in Fig. 1.

The functional form of Eqs. (2) and (4) is identical, up to replacing κ by λ, so the small nonzero bath polarization p affects the central spin in exactly the same way as the external field of the magnitude $H_0=-pAN/2$, equal to the average Overhauser field exerted on the central spin by the nuclear bath. Indeed, the noticeable average magnetization $\langle M\rangle=pN/2$ of the polarized bath leads to a noticeable average Overhauser field, but the variation of the magnetization $\langle(\Delta M)^2\rangle=(1-p^2)N/4$ changes very little at small p, and, correspondingly, the spread in the Overhauser fields is almost unchanged.

From Eqs. (2) and (4), we see that $\sigma_z(t)$ always decays with characteristic time $T_2^*=\sqrt{8/(NA^2)}$. E.g., for $H_0=0$ (or $p=0$), we reproduce a well-known result $\sigma_z(t)=(1/3)+(2/3)(1-Dt^2)\exp(-Dt^2/2)$, i.e., $\sigma_z(t)$ first falls to the value ≈0.036, then increases and saturates at $1/3$. However, for $H_0\neq0$ (or $p\neq0$), due to the oscillatory terms in Eq.

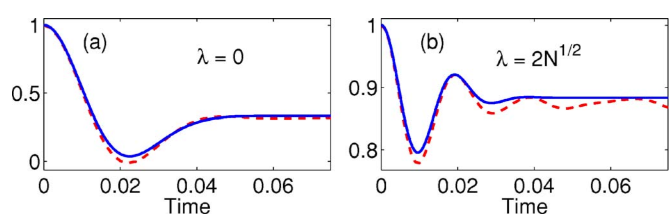

FIG. 2. (Color online) The same as Fig. 1 but for $N=2000$ nuclear bath spins in zero magnetic field (a) and in $\lambda=2\sqrt{N}$ (b) with initially unpolarized bath.

(3), $\sigma_z(t)$ can exhibit oscillations, provided that λ (or κ) is comparable or larger than $\sqrt{D}\sim\sqrt{N}$. This transition, from smooth decay at small field or polarization, to the oscillations at larger field or polarization, is similar to the well-known transition in the dynamics of a damped oscillator: the evolution of the central spin is overdamped (or underdamped) depending on whether the decay time T_2^* is larger (or smaller) than the "bare" oscillation frequency determined by λ or κ. Note that the crossover value for magnetic field (polarization) is of order of $\sqrt{N}$, beyond the range of applicability of the perturbation theory.[7,10]

For a typical GaAs QD with the electron delocalized over $N=10^6$ nuclear spins, $A\sim A_0/N\sim 10^{-4}$ μeV (where $A_0\approx 0.1$ meV is the hyperfine coupling for an electron localized on a single nucleus[24]). The corresponding decoherence time $T_2^*\sim 10$ ns (taking into account the $I=3/2$ spins of ^{69}Ga, ^{71}Ga, and ^{75}As), as confirmed by recent experiments.[1,19] To observe oscillations for a single electron spin, a very modest external field of order of 3 mT, or polarization of order of 0.5% is needed.

It is noteworthy that the decoherence time remains practically constant in the course of transition from smooth to oscillatory decay. The decoherence time is determined by the spread in the Overhauser fields, which is proportional to the variation of the bath magnetization $\langle(\Delta M)^2\rangle=(1-p^2)N/4$, and it is little affected by small bath polarizations p.[7,25] For a moderate bath polarization, the equivalence between the external field and the nonzero bath polarization disappears, and the analytical expression for $\sigma_z(t)$ becomes rather complex, involving hypergeometric functions $_2F_1(a,b,c,z)$ of a complex argument, so we do not present it here. In this regime, the decoherence time does not increase much, as shown in Figs. 1(e) and 1(f).

In order to substantially increase the decoherence time, an extremely large bath polarization is required, as suggested by the results from the perturbation method.[7–10] Such a large bath polarization is beyond the scope of our paper. Currently, strongly polarized baths are difficult to achieve experimentally, and such methods as narrowing the nuclear-spin distribution,[13] dynamical decoupling,[11] and spin-echo techniques[1,12] may be more practical for suppression of decoherence.

The quasistatic bath approximation is far from reality. E.g., for $H_0=0$ and $p=0$, the QSA predicts saturation of $\sigma_z(t)$ at 1/3 for $t\rightarrow\infty$, which is just an artifact of the approximation: the detailed analysis shows that σ_z slowly decays (as $1/\ln t$) to zero.[7,17,20] However, we expect QSA to be valid at times of order of T_2^*, when the bath's internal dynamics is not yet important.

For verification, we perform exact numerical simulation with medium-size baths of $N=20$ spins. A real QD is approximated by taking nuclear spins located at the sites of the 4×5 piece of a square lattice, with the lattice constant $a=1$. Assuming a parabolic confining potential, the electron density is approximated as two-dimensional (2D) Gaussian with the widths of $w_x=w_y=1.5$, and with the center shifted by $d_x=0.1$ and $d_y=0.29$ along the x and y axis, respectively. For comparison with the analytical results above, the effective coupling constant is defined as $A=(\Sigma_k A_k^2/N)^{1/2}$. The decoherence dynamics is simulated by directly solving the time-dependent Schrödinger equation for the wave function of the full many-spin system (central spin plus the bath), using the Chebyshev polynomial expansion of the evolution operator as described in Ref. 16.

Figures 1(a)–1(c) show analytical [obtained from Eq. (2)] and numerical results for $\sigma_z(t)$, for different magnetic fields. The panels (d)–(f) present $\sigma_z(t)$ for polarized baths with different initial polarizations. For the analytical curve in panel (d) the small-polarization formula Eq. (4) has been used, while the analytical curves in panels (e) and (f) have been calculated from the formula for moderate initial polarization. The agreement of the analytics and the exact numerics is good. The difference is caused only by the modest number $N=20$ of the bath spins used for numerical simulations, but exact simulations even for $N=50$ are beyond the capabilities of modern computers (since the computation time and memory grow exponentially with N).

To study large baths with $N=2000$, we use the coherent state P-representation described in Ref. 17. Although approximate, this numerical approach demonstrates excellent accuracy. Figure 2 presents the results for $\sigma_z(t)$ obtained analytically, from Eq. (2), and numerically, from P-representation simulations with $N=2000$ spins. For $N=2000$, the agreement between the analytics and the numerics is very good. Overall, the data presented in Figs. 1 and 2 justify the use of QSA, so that we expect our predictions to be valid for real QDs with 10^6 nuclear spins.

III. TWO ELECTRON SPINS IN DOUBLE QD

Measurement of the Rabi oscillations for a single electron spin in a QD has been achieved[26] only very recently, while the majority of recent experiments use two electron spins in two neighboring QDs.[1,19] The spins are prepared in the singlet state, and the measured quantity is the probability $P_S(t)$ to stay in the singlet state after time t. The oscillations described above can be also detected in this double-dot setup. When the coupling between the two electron spins is negligible, the Hamiltonian of the double-QD system is $\mathcal{H}=H_{01}S_{1z}+H_{02}S_{2z}+\Sigma_{j=1}^{N_1}A_j\mathbf{S}_1\cdot\mathbf{I}_j+\Sigma_{k=1}^{N_2}A_k\mathbf{S}_2\cdot\mathbf{I}_k$ where indices 1 and 2 denote the quantities describing left and right QD, respectively (e.g., H_{01} and H_{02} are the magnetic fields acting on the left and right spins, respectively). Note that the evolution of QD 1 and 2 is not independent because of the initially entangled singlet state, although the Hamiltonian is separable. Using the quasistatic approximation, we get

$$P_S=\frac{1}{2}U(\lambda_1,D_1)U(\lambda_2,D_2)+\frac{1}{2}W(\lambda_1,D_1)W(\lambda_2,D_2)+F(\lambda_1,D_1)F(\lambda_2,D_2)+G(\lambda_1,D_1)G(\lambda_2,D_2), \quad (5)$$

where the function $W(\lambda,D)$ is defined by Eq. (3), and $F(\lambda,D)=1/2\{1+[\cos\lambda t-(Dt/\lambda)\sin\lambda t]e^{-Dt^2/2}\}$, $G(\lambda,D)=1-F(\lambda,D)-W(\lambda,D)$, $U(\lambda,D)=(1/\lambda^2)[D\lambda t\cos\lambda t+(\lambda^2-D)\sin\lambda t]e^{-Dt^2/2}$. Figure 3(a) illustrates dynamics of $P_S(t)$ for unpolarized baths, in the case of uniform magnetic field $H_0=H_{01}=H_{02}$. $P_S(t)$ decays in the beginning, and satu-

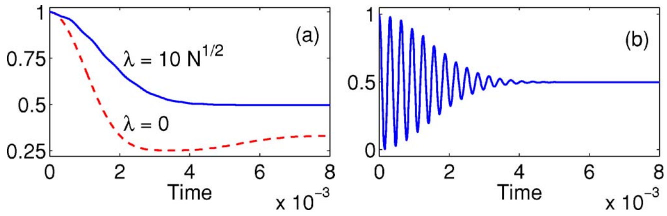

FIG. 3. (Color online) Time evolution of the probability of the singlet state of the two electrons in a double QD by applying (a) parallel magnetic fields $\lambda_1=\lambda_2=\lambda$ and (b) antiparallel magnetic fields $\lambda_1=-\lambda_2=10\sqrt{N}$ with $N_1=N_2=N=10^6$. Underdamped Rabi oscillations appear once the difference in the magnetic fields applied onto each QD is large enough.

rates at nonzero value at long times. The saturation value is 1/3 for zero field, and increases with the magnetic field, reaching 1/2 for strong fields.[19]

However, if the difference between H_{01} and H_{02} is comparable or larger than $A\sqrt{N_{1,2}}$ (which corresponds to few mT for realistic GaAs QD), the probability $P_S(t)$ exhibit oscillations [see Fig. 3(b)], analogous to the oscillations of $\sigma_z(t)$ in the single-QD case above. In experiments, a nonuniform magnetic field can be created, e.g., by micromagnets.[27] Another opportunity is using nonuniformly polarized nuclear-spin baths in the left and right QDs. In analogy to the single-QD calculations, it can be shown that $P_S(t)$ in the case of nonzero initial polarization is still given by Eqs. (5), with replacement of $\lambda_{1,2}$ by $\kappa_{1,2}$. The difference in polarization should be about 0.5% for the oscillations to appear.

IV. CONCLUSION

In summary, we study in detail the influence of magnetic fields and bath polarization on the decoherence of a single spin in a quantum dot, and two spins located in neighboring QDs. We focus on the regime of moderate fields and polarizations, where the perturbation theory is not yet applicable, using both analytical tools (the quasistatic bath approximation) and the numerical simulations (exact for medium-size baths with 20 spins, and approximate for large baths with 2000 spins). The agreement between all three approaches is good, so we believe our results are applicable to real QDs with millions of nuclear spins. The nonzero bath polarization and the external magnetic field influence the decoherence dynamics in exactly the same way, and lead to a transition from smooth decay to oscillations once the field (polarization) exceeds a certain crossover value. This transition can be observed in experiments with a single QD, and with two quantum dots. Our results show that a substantial increase of the decoherence time requires extremely large bath polarizations, so that such methods as dynamical decoupling[1,11,12] or control of the nuclear-spin distribution[13] may be more practical for controlling decoherence of QD-based qubits.

ACKNOWLEDGMENTS

This work was supported by the NSA and ARDA under Army Research Office (ARO) Contract No. DAAD 19-03-1-0132. This work was partially carried out at the Ames Laboratory, which is operated for the U. S. Department of Energy by Iowa State University under Contract No. W-7405-82 and was supported by the Director of the Office of Science, Office of Basic Energy Research of the U. S. Department of Energy. K.A.A. and E.D. were supported by NSF Grant No. DMR-0454504.

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