Control of a two-electron double quantum dot with an external magnetic field

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We investigate the utilization of external magnetic field for the manipulation of the quantum states in a two-electron double quantum dot. The singlet and triplet states are coupled through the hyperfine interaction between the electrons and surrounding nuclei. When the magnetic field is changed as a function of time, the singlet-triplet transition is possible for certain values of magnetic field, when the singlet state becomes degenerate with the triplet state. The transition probability depends on the sweeping speed of the magnetic field through the averaged Landau-Zener formula. We evaluate proper time scales for efficient control of the quantum dot, evaluate the singlet probabilities for different time-dependent magnetic fields, and study the average of the final singlet probability, averaged over the orientations of the nuclear spins surrounding the quantum dot.

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I. INTRODUCTION

A setup of electrons confined in quantum dots[1] has emerged during recent years as one of the most interesting alternatives for quantum computing architecture.[2–4] For the construction of a working quantum computer, complete control of the qubit must be achieved in order to enable successful performance of quantum operations. For the time being, several alternative control schemes have been studied. The control of a single-electron quantum dot has been performed using resonant radio-frequency electrical pulses,[5] ultrafast optical pulses,[6,7] and by manipulating the dot shape using electric fields.[8] Theoretical investigations of the control of single-electron quantum dots have been made on optimized laser pulses,[9,10] photon polarization,[11] and by manipulating the electric field.[12]

For two-electron double quantum dots, control has been realized by manipulating the exchange interaction using electric fields,[13] which may be used to construct quantum gates.[14] Recently there have been studies of control schemes for two-electron double quantum dots regarding microwave pulses[15] and the use of time-dependent electric fields in order to produce desired final state for the quantum dot.[16,17] A control scheme for double quantum dot, which enables control of the nuclear polarization in the vicinity of the quantum dot, has also been presented.[18]

In this paper, we study the control of a two-electron double quantum dot using magnetic field. The lowest-lying energy states of the two-electron double quantum dot are the singlet state $|S\rangle$ and the triplet states $|T_-\rangle$, $|T_0\rangle$, and $|T_+\rangle$. The singlet state has degeneracy points with all or some triplet states, depending on the interdot distance (see Fig. 1). In a GaAs quantum dot, the hyperfine interaction between the spins of the electrons in the quantum dot and the spins of the surrounding nuclei couples the singlet and triplet states at the degeneracy points. By varying the sweeping speed of the magnetic field over the degeneracies, the final state of the double quantum dot may be controlled. Depending on the sweeping speed, the transitions at the singlet-triplet degeneracy points are diabatic, adiabatic, or a combination of both these possibilities. This behavior is explained by the Landau-Zener formula.[19–21] We analyze the system using a 4×4 Hamiltonian matrix, derived by Coish and Loss,[22] and evaluate numerically the probabilities of the singlet and triplet states as a function of time. In addition, we calculate the final singlet probability as a function of the sweeping time for a single singlet-triplet transition using the Landau-Zener formula and average it over the hyperfine field realizations.

II. MODEL

We model the two-electron system with the Hamiltonian

$$H=\sum_{i=1}^{2}\left(\frac{\left(-i\hbar\nabla_i-\frac{e}{c}\mathbf{A}_i\right)^2}{2m^*}+V(\mathbf{r}_i,\mathbf{s}_i)\right)+\frac{e^2}{\epsilon r_{12}}, \qquad (1)$$

where the effective mass $m^*=0.067m_e$ and permeability $\epsilon=12.7$ are material parameters for GaAs. The external potential V is a sum of two different potentials,

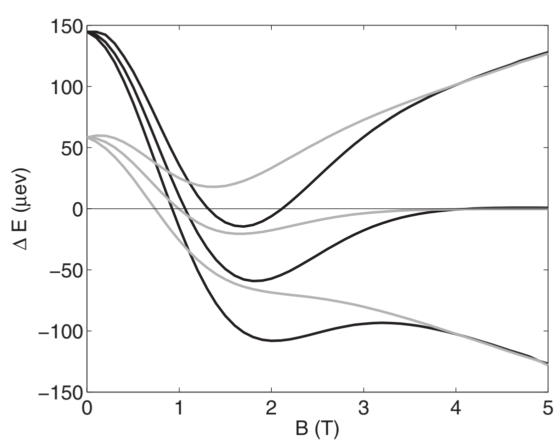

FIG. 1. The energy difference ΔE between the singlet state S and triplet states T_-, T_0, and T_+ as a function of the external magnetic field. In the calculation of these energies, the hyperfine field is set to zero. The dark (light) gray lines correspond to dot distance 40 (50) nm.

$$V = V_C + V_Z. \tag{2}$$

The first part in the external potential is a two-minima parabolic confinement potential

$$V_C(\mathbf{r}) = \frac{1}{2}m^*\omega_0^2 \min\left[\sum_{j=1}^{2}(\mathbf{r}-\mathbf{L}_j)^2\right], \tag{3}$$

where the confinement strength is $\hbar\omega_0=3.0$ meV and $\mathbf{L}_j$ give the positions of the minima of the confinement potential. The second part, V_Z, is the potential caused by the Zeeman interaction

$$V_Z(\mathbf{r},\mathbf{s}) = g^*\mu_B\mathbf{B}(\mathbf{r})\cdot\mathbf{s}, \tag{4}$$

where the Lande factor of GaAs is $g^*=-0.44$. The magnetic field can be divided into a homogeneous external magnetic field $\mathbf{B}_{\text{ext}}$ and an inhomogeneous random hyperfine field $\mathbf{h}(\mathbf{r})$.

We discretize the Hamiltonian using finite difference method and determine its eigenvalues using Lanczos diagonalization. The difference between the energies of the singlet and triplet states is denoted with ΔE. The strength of the hyperfine field $\mathbf{h}$ is determined from a fit to singlet-triplet decoherence measurements.[23,24] The eigenenergies of the singlet and triplet states depend on the external magnetic field. In Fig. 1, the energy differences between the singlet and triplet states are shown as a function of the magnetic field for two dot distances, 40 and 50 nm. As the magnetic field increases, the energy differences diminish and for the 40 nm distance, all three energy differences change sign. This means that the singlet state has a degeneracy with all the triplet states, making a transition from singlet state to triplet states possible. For larger distances, the exchange energy is smaller. Then the Zeeman term is dominant and the $|S\rangle-|T_+\rangle$ energy difference does not change sign. Finally, when the distance is so large that the exchange energy vanishes, the energies depend linearly on the magnetic field as the energy difference is given by the Zeeman energy.

In this setup, the energies of the states above the four lowest-lying states are considerably larger than their coupling with the lowest-lying states induced by the hyperfine field. Hence, we approximate the dynamics of the system using a 4×4 Hamiltonian, constructed on the basis of the singlet and three triplet states. For brevity, we introduce variables[22] that depend on the hyperfine fields around the two electrons $h_{1,2}$

$$h^i = \frac{1}{2}(h_1^i + h_2^i), \quad \delta h^i = \frac{1}{2}(h_1^i - h_2^i), \tag{5}$$

$$h^{\pm} = h^x \pm ih^y, \quad \delta h^{\pm} = \delta h^x \pm i\delta h^y. \tag{6}$$

Using these variables, the Hamiltonian matrix H_{eff} takes the form[22]

$$\begin{pmatrix} 0 & -\delta h^+/\sqrt{2} & \delta h^z & \delta h^-/\sqrt{2} \\ -\delta h^-\sqrt{2} & J+\epsilon_Z+h^z & h^-/\sqrt{2} & 0 \\ \delta h^z & h^+/\sqrt{2} & J & h^-/\sqrt{2} \\ \delta h^+/\sqrt{2} & 0 & h^+/\sqrt{2} & J-\epsilon_Z-h^z \end{pmatrix},$$

where $\epsilon_Z=g^*\mu_B B^z$.

III. SPIN DYNAMICS

A. Generalized Landau-Zener approach

We analyze the evolution of the system when the magnetic field is swept over such values that each triplet eigenenergy becomes degenerate with the singlet state. In the vicinity of the crossing points of the singlet and triplet energies, the dynamics of the system is effectively described by a 2×2 Hamiltonian on the basis of the crossing singlet and triplet states

$$H = \begin{pmatrix} 0 & \delta \\ \delta & \Delta E \end{pmatrix}, \tag{7}$$

where δ is the off-diagonal matrix element coupling the degenerate singlet and triplet states and ΔE is the energy difference between these states. Because the coupling is typically small, we may use perturbation theory and the matrix elements are calculated from space integrals, e.g., in the case of $|S\rangle-|T_0\rangle$ crossing,

$$\delta = \langle S|H_{hf}|T_0\rangle = \frac{1}{2}\int\int d\mathbf{r}_1 d\mathbf{r}_2 \psi_S^*(\mathbf{r}_1,\mathbf{r}_2) \times (B_1^z - B_2^z)\psi_T(\mathbf{r}_1,\mathbf{r}_2). \tag{8}$$

The wave function ψ is expressed using the expansion coefficients of the degenerate states α_1 and α_2 as

$$\psi = \begin{pmatrix} \alpha_1 \\ \alpha_2 \end{pmatrix}. \tag{9}$$

From the Schrödinger equation (we denote $\hbar=1$) $i\frac{\partial\psi}{\partial t}=H\psi$, we obtain a differential equation for α_1,

$$-\frac{1}{\delta}\frac{\partial^2\alpha_1}{\partial t^2} = \delta\alpha_1 + i\frac{\Delta E}{\delta}\frac{\partial\alpha_1}{\partial t}. \tag{10}$$

When the magnetic field is changed as a function of time, the time dependence of the energy difference $\Delta E(t)$ is rather complicated (see Fig. 1), making this differential equation difficult to solve. However, the hyperfine coupling of the singlet and triplet states is weak. Thus, the singlet probability changes only in the vicinity of the singlet-triplet degeneracy, where we may approximate $\Delta E(t)$ using a linear function $\Delta E=Kt$. Substituting $\Delta E=Kt$, we get the differential equation

$$\frac{\partial^2\alpha_1}{\partial t^2} + iKt\frac{\partial\alpha_1}{\partial t} + \delta^2\alpha_1 = 0. \tag{11}$$

Starting from the singlet state, having initial condition $|\alpha_1(t=-\infty)|^2=1$, we evaluate the asymptotic value of the singlet probability $|\alpha_1(t=\infty)|^2$. We do not have to solve this differ-

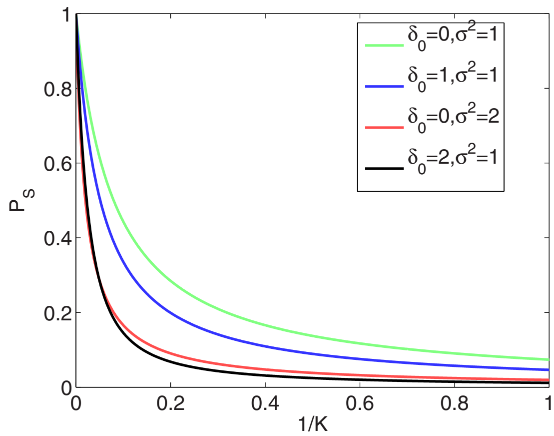

FIG. 2. (Color online) Probabilities P_S of the singlet state S as a function of the inverse of the time derivative K of the energy difference for different values of the mean δ_0 and variance σ^2 of the hyperfine field.

ential equation in order to obtain it, as the asymptotic probability is given by the famous Landau-Zener formula for nonadiabatic transitions[19–21]

$$|\alpha_1(t=\infty)|^2 = \exp\left(-\frac{2\pi\delta^2}{|K|}\right). \quad (12)$$

The finite temperature of the hyperfine spins causes fluctuations in the random hyperfine field. Thus, a measurement of the singlet probability is effectively made over an ensemble of different hyperfine fields. Hence, it is interesting to calculate the average of the asymptotic singlet probability over the hyperfine-field realizations. We define the off-diagonal element δ as a randomly distributed complex number, having mean δ_0 and variance σ^2. Both the real and imaginary parts of δ are normally distributed, hence we obtain the average of the singlet probability $\langle P_S\rangle$ from the integral [we denote $x=\mathrm{Re}(\delta)$ and $y=\mathrm{Im}(\delta)$]

$$\langle P_S\rangle = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\exp\left[-\frac{(x-x_0)^2}{2\sigma^2}\right]\exp\left[-\frac{(y-y_0)^2}{2\sigma^2}\right] \times\exp\left[-\frac{2\pi(x^2+y^2)}{|K|}\right]dxdy, \quad (13)$$

which gives

$$\langle P_S\rangle = \exp\left(-\frac{2\pi|\delta_0|^2}{|K|+4\pi\sigma^2}\right)\frac{1}{1+4\pi\frac{\sigma^2}{|K|}}. \quad (14)$$

One can see, that the Gaussian form of Landau-Zener formula is modified and multiplied with a Lorentzian function.

Figure 2 illustrates the asymptotic singlet probabilities for different values of the mean and variance of the hyperfine field as a function of $1/K$, where K is the time derivative of the energy difference. The singlet probability diminishes rapidly as the slope of the energy difference decreases, because the slow change in the energy difference keeps the energy difference longer in the vicinity of zero, enabling the decay of the singlet state. If either the polarization or the variance of the hyperfine field is increased, resulting curves have similar shapes, as the two lowermost curves in Fig. 2 indicate. This makes it difficult to determine the hyperfine field polarization from the measurements.[25]

We calculate the variance of the asymptotic singlet probability in a similar fashion as above, using the relation $\sigma^2(P_S)=\langle P_S^2\rangle-\langle P_S\rangle^2$, which yields

$$\sigma^2(P_S) = \exp\left(-\frac{4\pi|\delta_0|^2}{|K|+8\pi\sigma^2}\right)\frac{1}{1+8\pi\frac{\sigma^2}{|K|}} - \exp\left(-\frac{4\pi|\delta_0|^2}{|K|+4\pi\sigma^2}\right)\frac{1}{\left(1+4\pi\frac{\sigma^2}{|K|}\right)^2}. \quad (15)$$

We observe that the variance approaches zero in the limits $|K|\to 0$ and $|K|\to\infty$.

B. Numerical analysis

In the following, we study the evolution of the quantum dot states by using numerical methods. The wave function of the system is written on the basis of the four singlet and triplet states, and the singlet and triplet probabilities are calculated from the squares of the absolute values of the respective basis functions. We calculate numerically the wave function of the system using the relation $\psi(t)=\exp(-iH_{\mathrm{eff}}t)\psi(0)$. The magnetic field is changed linearly as a function of time, which causes a time dependence in the energy difference (see Fig. 1). Due to this, the effective Hamiltonian changes at each time step. The magnetic field is changed rapidly (in 55 μs) in Fig. 3(a) and slowly (in 550 μs) in Fig. 3(b). The distance of the dots is 40 nm, which makes all three singlet-triplet transitions possible. Figure 3 shows that the probability of the singlet state changes very rapidly when the $|S\rangle-|T_-\rangle$ crossing point is reached. Once the energy difference has changed sign and its absolute value increases, the decrease in the singlet probability stops and it remains constant. Similar stepwise decrease is observed at the $|S\rangle-|T_0\rangle$ and $|S\rangle-|T_+\rangle$ crossing points. The probabilities of the triplet states $|T_0\rangle$, $|T_+\rangle$, whose crossing point is reached later, have a smaller probability than $|T_-\rangle$ state, because the singlet probability diminishes and the conservation of the total probability restricts the probabilities of the other triplet states. We notice that the time interval of the singlet-triplet transitions is less than 1 μs. The value of the off-diagonal matrix element, which couples the respective singlet and triplet states, effects the spin dynamics only during the transition. Outside the transition points, the nonzero singlet-triplet energy difference does not allow transition. As the time scale of the fluctuations of the hyperfine field is around 10–100 μs,[4] the off-diagonal matrix elements may be considered constant during the simulation. The value of each off-diagonal matrix element should be interpreted to be the value the element has at the moment of the singlet-triplet transition.

If the magnetic field is changed rapidly [Fig. 3(a)], the energy difference is in the vicinity of zero for a shorter time. Thus, the singlet probability does not have time to change

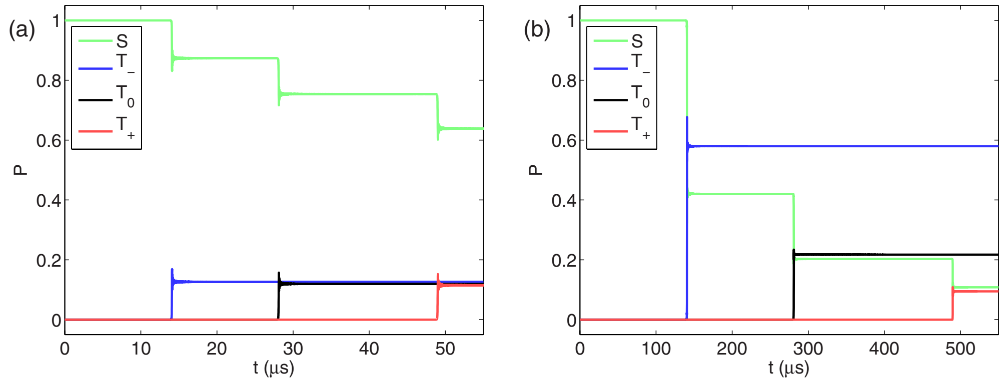

FIG. 3. (Color online) Probabilities P of the singlet state S and triplet states T_-, T_0, and T_+ as a function of time averaged over 1000 realizations. In the left (right) figure the magnetic field is switched from 0.75 to 1.35 T in 55 (550) μs. Distance of the dots is 40 nm.

much, making the steps of the singlet probability smaller. The oscillations of the singlet and triplet states are invisible in Fig. 3, because the damping of the oscillations is remarkably fast. Only the peaks at the singlet-triplet crossing points are observed. In Fig. 1, the slopes for the energy differences $|S\rangle - |T_0\rangle$ and $|S\rangle - |T_+\rangle$ are smaller than for $|S\rangle - |T_-\rangle$, which would give these triplet states larger probabilities according to Eq. (14) but the remaining singlet probabilities before the respective singlet-triplet crossings are smaller, which limits the value of the triplet probability giving these states almost equal probabilities. If the distance of the dots is increased to 50 nm, the $|S\rangle - |T_+\rangle$ energy difference is always positive. Hence, there would be only two steps of the singlet probability in this case and the probability of the $|T_+\rangle$ state would remain zero. We may choose different velocities for different singlet-triplet crossings, and by crossing certain point slowly, and another point rapidly we may produce various final states for the quantum dot.

For different realizations, the time dependence of the singlet and triplet probabilities varies considerably. The values of the singlet probabilities during the magnetic-field sweeping for a large number of realizations are represented in Fig. 4. The three different times, for which the probability distribution is shown, are selected to be after each Landau-Zener transition. In Fig. 4(b), all probability distributions have a peak at $P_S=0$, because for slower transition there is a large probability for total disappearance of the singlet probability. The probabilities of the second and third transition are restricted by the probability after the first transition, which naturally cannot be exceeded. In Fig. 4(a), the peaks of the distributions are closer to $P_S=1$. As in Fig. 4(b), the distributions of the probabilities after two or three transitions have a flatter shape than the first due to the conservation of the total singlet probability. The forms of these three distributions resemble the gamma distribution. The Landau-Zener transition has an analogy with a Poisson process, where δ^2 corresponds to the event probability in a time unit. Gamma distribution is related to probabilities of several independent Poissonian events. In our case, the Landau-Zener transitions are not independent of each other, because the total change in the probability is restricted to 1. In the faster magnetic-field sweeping, this restriction has smaller effect on the probability distribution and the shapes of the distributions are quite close to gamma distributions.

As Fig. 3 shows, the value of the singlet probability after the sweeping of the magnetic field depends strongly on the speed of the process. We calculate the singlet probability in the case where the magnetic field is changed from 0.75 to 0.95 T in time τ (interdot distance is 40 nm and the hyperfine field has zero mean). Now only the $|S\rangle - |T_-\rangle$ degeneracy point is crossed. Because there is only one singlet-triplet transition, the asymptotic singlet probability is given by Eq.

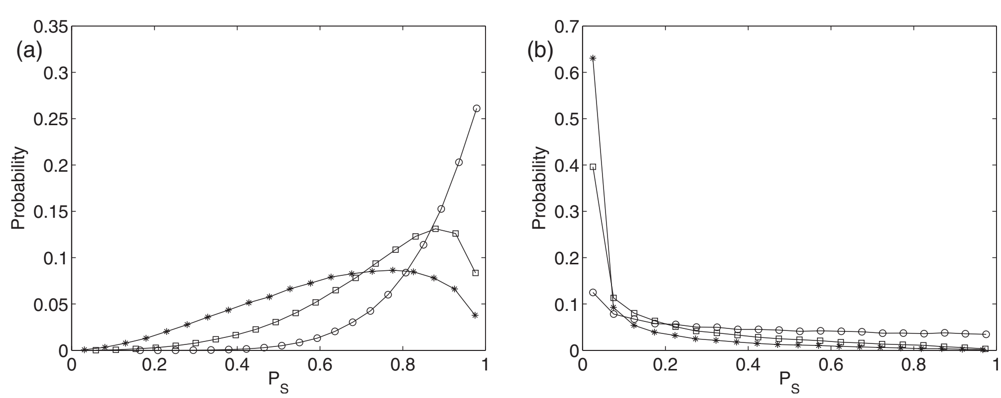

FIG. 4. The probability distribution of the singlet probability P_S for large collection of nuclear-field realizations. Panel (a) is for the case shown in Fig. 3(a) and (b) is for Fig. 3(b). The times are 22 (220) μs for circles, 39 (390) μs for squares, and 55 (550) μs for asterisks. The data points are connected with lines for clarity.

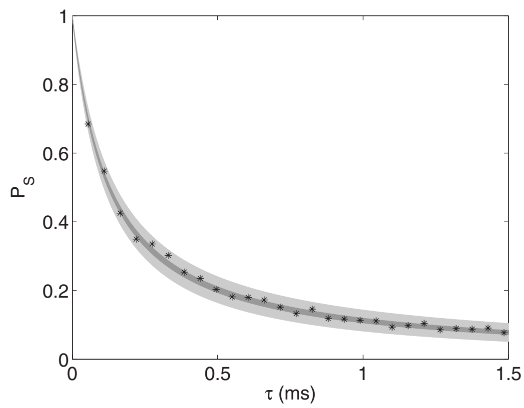

FIG. 5. The asymptotic singlet probability P_S, indicated with markers, as a function of the switching time τ of the magnetic field. The light (dark) gray area gives the range of the asymptotic values inside the standard error of the mean of 50 (1000) realizations.

(14) and its variance by Eq. (15), where $\delta_0=0$. Figure 5 shows the asymptotic singlet probability as a function of τ, averaged over 1000 realizations. The shadings in Fig. 5 indicate the mean given by Eq. (14) and the variance of the mean, obtained from Eq. (15) for 50 and 1000 realizations. The numerical values of the asymptotic singlet probability are situated inside the light-gray area and roughly half of the points inside the dark-gray area as should. We can see that the change in the magnetic field from 0.75 to 0.95 T should be made in 0.1–1.0 ms in this setup in order to have singlet probabilities that differ from 0 and 1. If the sweeping is faster than 0.1 ms, the singlet probability does not have time to change. For sweeping times larger than 1 ms, the singlet probability approaches zero. The variance has a maximum around $\tau=0.2$ ms, for larger τ variance diminishes slightly.

IV. SUMMARY

In summary, we have studied control of a two-electron double quantum dot using external magnetic field. We calculated the eigenenergies of the four lowest-lying (singlet and three triplet) states and analyzed the evolution of the singlet and triplet states of the quantum dot. We used a 2×2 matrix model Hamiltonian, which led to a second-order differential equation for the singlet probability. The transition probability from the singlet state to the triplet state was obtained from the Landau-Zener formula. Numerical simulations of the evolution of the states showed that the singlet probability changes only at the vicinity of the singlet-triplet crossing and behaves according to the Landau-Zener formula. We analyzed the distribution of the singlet probability for different realizations and the dependence of the final singlet probability on the sweeping speed of the external magnetic field. Our results indicate, that the quantum states of the double quantum dot can be controlled by applying time-dependent external magnetic field.

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