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

J. Särkkä and A. Harju

Department of Applied Physics and Helsinki Institute of Physics, Helsinki University of Technology, P.O. Box 4100, Espoo, FI-02015 TKK, Finland

(Received 17 October 2008; revised manuscript received 17 December 2008; published 20 February 2009)

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.

DOI: 10.1103/PhysRevB.79.085313 PACS number(s): 73.21.La, 71.70.Gm, 71.70.Jp

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[1] has emerged during recent years as one of the most interesting alternatives for quantum computing architecture.[2–5] In low temperatures, the most significant decoherence source is the hyperfine interaction of the electrons with the surrounding nuclear spins.[6–9] There are several methods to suppress the decoherence induced by the hyperfine field. The narrowing of the hyperfine field distribution is one method.[10] This is realized, e.g., by gate-controlled Rabi oscillations[11] or by optical preparation of nuclear spins.[12] The polarization of the nuclear spins could also diminish the decoherence rate,[2] but nearly 100% polarization is required,[10] which is presently not feasible. However, the decoherence time may be substantially increased by a nuclear-spin pumping cycle, which suppresses the hyperfine field fluctuation by a factor of 70.[13,14] 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.*[15] 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,[16] where they describe the system using a 2×2 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[16]

$$H = \epsilon_z(S_1^z + S_2^z) + \mathbf{h}_1\cdot\mathbf{S}_1 + \mathbf{h}_2\cdot\mathbf{S}_2 - J\left(\tfrac{1}{4} - \mathbf{S}_1\cdot\mathbf{S}_2\right), \quad (1)$$

where $\mathbf{S}_{1,2}$ are the spin operators of the electrons, $\mathbf{h}_{1,2}$ are the hyperfine fields the electrons interact with, ϵ_z is the Zeeman energy, and J is the exchange energy. We write the Hamiltonian in a more compact form

$$H = \epsilon_z S^z + \mathbf{h}\cdot\mathbf{S} + \delta\mathbf{h}\cdot\delta\mathbf{S} + \frac{J}{2}\mathbf{S}\cdot\mathbf{S} - J, \quad (2)$$

where $\mathbf{h}=\mathbf{h}_1+\mathbf{h}_2$, $\mathbf{S}=\mathbf{S}_1+\mathbf{S}_2$, $\delta\mathbf{h}=\mathbf{h}_1-\mathbf{h}_2$, and $\delta\mathbf{S}=\mathbf{S}_1-\mathbf{S}_2$. 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,[9,15] as our numerical simulations using realistic parameters from these experiments show that the two triplet states with $S_z=\pm 1$ remain unoccupied.[17] 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

$$H = \frac{J}{2}\mathbf{S}\cdot\mathbf{S} + \delta h^z \delta S^z, \quad (3)$$

which in matrix form reads

$$H = \begin{pmatrix} 0 & \delta h^z \\ \delta h^z & J \end{pmatrix}. \quad (4)$$

The exact time dependence of the wave function can be calculated from the relation $\psi(t)=\exp(-iHt/\hbar)\psi(0)$. We denote $\psi(t)=(\alpha(t)\beta(t))^T$ and use the initial condition $\psi(0)=(10)^T$. We obtain the coefficient $\alpha(t)$ from the relation,

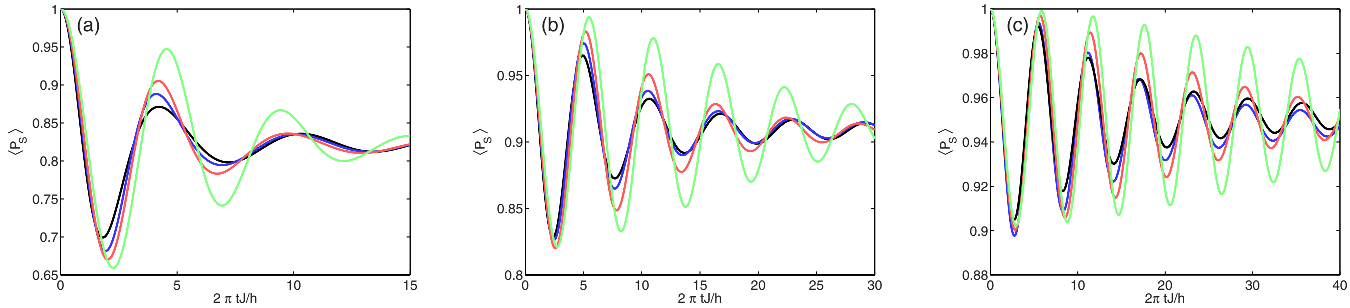

FIG. 1. (Color online) Singlet probability $\langle P_S \rangle$ as a function of time in the cases (a) $\langle P_S(\infty)\rangle = 0.82$, (b) 0.91, and (c) 0.95, correspondingly. The values of the mean and standard deviation used in each curve are given in the Table I. The amplitude of the oscillation increases with the polarization of the hyperfine field h_0.

$$\alpha(t) = \psi(0)^T A \begin{pmatrix} \exp(i\lambda_1 t) & 0 \\ 0 & \exp(i\lambda_2 t) \end{pmatrix} A^{-1}\psi(0), \qquad (5)$$

where $\lambda_{1,2} = \frac{1}{2}(J \pm \sqrt{4(\delta h^z)^2 + J^2})$ 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

$$P_S(t) = \frac{1}{2}\left[1 + \frac{J^2}{D^2} + \left(1 - \frac{J^2}{D^2}\right)\cos(Dt)\right], \qquad (6)$$

where $D = \sqrt{4(\delta h^z)^2 + J^2}$. For constant δh^z, the singlet probability oscillates sinusoidally. In order to obtain the average over the statistical ensemble of hyperfine spins, we assume the coupling δh^z to be normally distributed with mean h_0 and variance σ_0^2. The ensemble average of the singlet probability as a function of time over the hyperfine field is given by

$$\langle P_S(t)\rangle = \frac{1}{\sqrt{2\pi}\sigma_0}\int_{-\infty}^{\infty} \exp\left(-\frac{(\delta h_z - h_0)^2}{2\sigma_0^2}\right) P_S(t) d(\delta h_z).$$

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 h_0 and variance σ_0^2 on the singlet probability $\langle P_S(t)\rangle$.

B. Spin oscillation

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 σ_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.[17] 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] were able to 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/σ_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 av-

TABLE I. The values of the mean h_0 and standard deviation σ_0 and colors (gray scales) of the respective curves in Fig. 1.

P_S	h_0/J	σ_0/J	Color (gray scale)
0.820	0	0.526	Black
	0.365	0.316	Blue (dark gray)
	0.379	0.263	Red (middle gray)
	0.384	0.158	Green (light gray)
0.910	0	0.277	Black
	0.203	0.166	Blue (dark gray)
	0.215	0.139	Red (middle gray)
	0.229	0.083	Green (light gray)
0.950	0	0.183	Black
	0.126	0.128	Blue (dark gray)
	0.149	0.092	Red (middle gray)
	0.161	0.055	Green (light gray)

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),

$$\bar{P}_S = \frac{1}{2}\left(1 + \frac{J^2}{D^2}\right). \tag{7}$$

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,

$$\langle \bar{P}_S \rangle = \frac{1}{2\sqrt{2\pi}\sigma_0}\int_{-\infty}^{\infty} \exp\left(-\frac{(\delta h_z - h_0)^2}{2\sigma_0^2}\right)\bar{P}_S, \tag{8}$$

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

$$\langle \bar{P}_S \rangle = \frac{1}{2} + \sqrt{\frac{\pi}{2}}\frac{J}{4\sigma_0}\exp\left(\frac{J^2 - 4h_0^2}{8\sigma_0^2}\right) \times \mathrm{Re}\left[\exp\left(\frac{iJh_0}{2\sigma_0^2}\right)\mathrm{erfc}\left(\frac{J + 2ih_0}{2\sqrt{2}\sigma_0}\right)\right]. \tag{9}$$

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

$$\langle \bar{P}_S \rangle = \frac{1}{2} + \sqrt{\frac{\pi}{2}}\frac{J}{4\sigma_0}\exp\left(\frac{J^2}{8\sigma_0^2}\right)\mathrm{erfc}\left(\frac{J}{2\sqrt{2}\sigma_0}\right). \tag{10}$$

When the standard deviation σ_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 $\delta h_z = h_0$ and we have

$$\langle \bar{P}_S \rangle = \frac{1}{2}\left(1 + \frac{1}{4\left(\frac{h_0}{J}\right)^2 + 1}\right). \tag{11}$$

The exchange energy J gives the relevant energy scale of the system. Thus, it is natural to measure h_0 and σ_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 δh^z 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 the mean constant, the hyperfine field starts to have more values in the vicinity of zero, and as a result of this, decoherence is weaker and the triplet probability has a minimum. For $\frac{h_0}{J} > 0.5$, the minimum point is around $\frac{3}{5}h_0 < \sigma_{\min} < h_0$. For $\frac{h_0}{J} \gg 1$, minimum is at $\sigma_{\min} \approx h_0$. As the standard deviation is still increased, hyperfine field has more values far from zero. This strengthens the decoherence and the triplet probability goes toward the limit $\frac{1}{2}$. If the fluctuations of the hyperfine field are suppressed,[14] the asymptotic value of the triplet probability depends strongly on the polarization of the hyperfine field. This would be one alternative for experimental polarization studies.

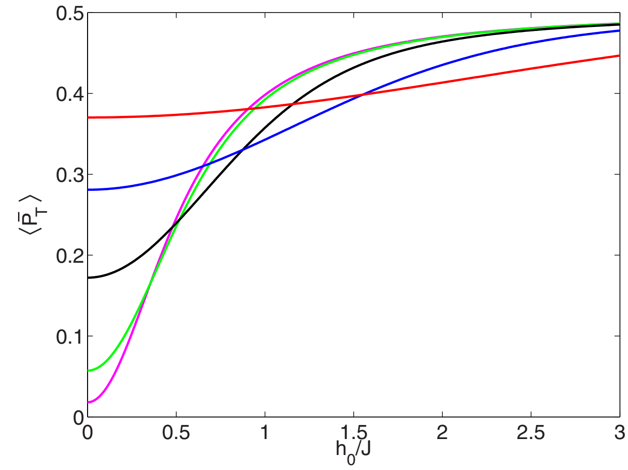

FIG. 2. (Color online) Asymptotic triplet probability $\langle \bar{P}_T \rangle$ as a function of the mean of the hyperfine field $\frac{h_0}{J}$ for different values of the standard deviation of the hyperfine field. From bottom to top at $h_0=0$: $\frac{\sigma_0}{J}=0.1$, 0.2, 0.5, 1.0, and 2.0.

The variance of the asymptotic singlet probability $\sigma^2(\langle \bar{P}_S \rangle)$ may be easily calculated using similar method as with the derivation of the formulas for $\langle \bar{P}_S \rangle$. Now we also have to calculate the average of the square of the mean $\bar{P}_S^2$

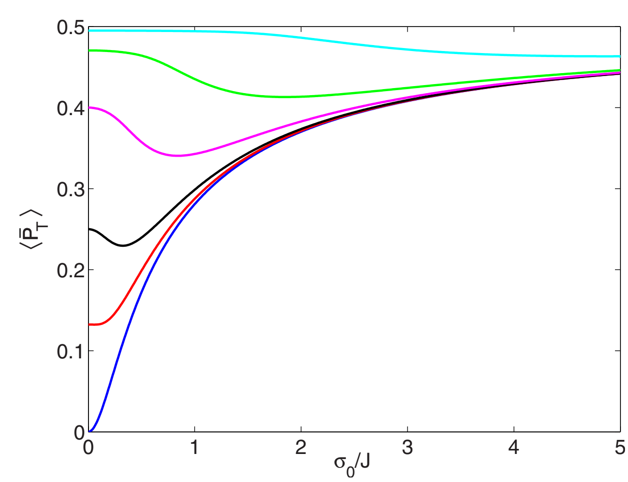

FIG. 3. (Color online) Asymptotic triplet probability $\langle \bar{P}_T \rangle$ as a function of the of the standard deviation of the hyperfine field $\frac{\sigma_0}{J}$ for different values of the mean of the hyperfine field. From bottom to top: $\frac{h_0}{J}=0$, 0.3, 0.5, 1.0, 2.0, and 5.0.

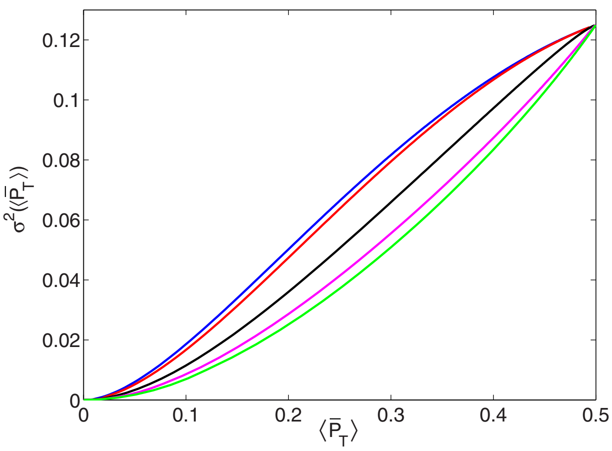

FIG. 4. (Color online) Asymptotic variance of the triplet probability $\sigma^2(\langle \bar{P}_T \rangle)$ as a function of the asymptotic triplet probability $\langle \bar{P}_T \rangle$ for different values of ratio of the mean and variance of the hyperfine field. From top to bottom: $\frac{h_0}{\sigma_0}=0$, 1.0, 2.0, 3.0, and 4.0.

and use the relation $\sigma^2(\langle \bar{P}_S \rangle)=\langle \bar{P}_S^2 \rangle - \langle \bar{P}_S \rangle^2$. The results of the derivation are given in the Appendix.

In an experimental setup, the parameter that may easily be adjusted is the exchange energy J. The hyperfine field distribution is typically frozen on the relevant time scale here. It is therefore interesting to depict the situation using the dimensionless ratio $r_0=\frac{h_0/J}{\sigma_0/J}=\frac{h_0}{\sigma_0}$, which does not depend on J. The asymptotic variance $\sigma^2(\langle \bar{P}_T \rangle)$ as a function of the asymptotic singlet probability $\langle \bar{P}_T \rangle$ for different ratios r_0 is drawn in Fig. 4. As the ratio r_0 increases, the variance of the triplet probability decreases. For $r_0 > 4$, the curves change only very slightly with increasing r_0. This data could be used to obtain information on the shape of the hyperfine field distribution. This is done by measuring the asymptotic triplet probability and its variance. Thus, it is possible to find the curve which intersects with the corresponding measurement point and determine r_0. However, the asymptotic variance does not vary much with the ratio r_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

This work has been supported by Academy of Finland through its Centers of Excellence Program (2006–2011). J.S. acknowledges financial support from the Finnish Cultural Foundation.

APPENDIX: VARIANCE OF THE ASYMPTOTIC SINGLET PROBABILITY

For the time average of the squared singlet probability $\bar{P}_S^2=\frac{1}{T}\int_0^T P_S(t)^2 dt$, 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 $\sigma^2(\langle \bar{P}_S \rangle)=\langle \bar{P}_S^2 \rangle - \langle \bar{P}_S \rangle^2$,

$$\sigma^2(\langle \bar{P}_S \rangle) = \frac{1}{64}\left(8 + 3\frac{J^2}{\sigma_0^2} - \sqrt{2\pi}\exp\left(\frac{J^2-4h_0^2}{8\sigma_0^2}\right)\left\{\frac{J}{\sigma_0}\mathrm{Re}\left[\exp\left(\frac{iJh_0}{2\sigma_0^2}\right)\mathrm{erfc}\left(\frac{J+2ih_0}{2\sqrt{2}\sigma_0}\right)\right] + \sqrt{2\pi}\frac{J^2}{\sigma_0^2}\exp\left(\frac{J^2-4h_0^2}{8\sigma_0^2}\right)\right.\right.$$
$$\left.\left.\times\left\{\mathrm{Re}\left[\exp\left(\frac{iJh_0}{2\sigma_0^2}\right)\mathrm{erfc}\left(\frac{J+2ih_0}{2\sqrt{2}\sigma_0}\right)\right]\right\}^2 + \frac{3J^3}{4\sigma_0^3}\mathrm{Re}\left[\exp\left(\frac{iJh_0}{2\sigma_0^2}\right)\left(2i\frac{h_0}{J}+1\right)\mathrm{erfc}\left(\frac{J+2ih_0}{2\sqrt{2}\sigma_0}\right)\right]\right\}\right).$$

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

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

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

$$\sigma^2(\langle \bar{P}_S \rangle) = \frac{1}{8}\left(1 - \frac{2}{4\left(\frac{h_0}{J}\right)^2+1} + \frac{1}{\left[4\left(\frac{h_0}{J}\right)^2+1\right]^2}\right).$$

[1] D. Loss and D. P. DiVincenzo, Phys. Rev. A **57**, 120 (1998).

[2] G. Burkard, D. Loss, and D. P. DiVincenzo, Phys. Rev. B **59**, 2070 (1999).

[3] J. M. Taylor, H.-A. Engel, W. Dür, A. Yacoby, C. M. Marcus, P. Zoller, and M. D. Lukin, Nat. Phys. **1**, 177 (2005).

[4] R. Hanson and G. Burkard, Phys. Rev. Lett. **98**, 050502 (2007).

[5] R. Hanson, L. P. Kouwenhoven, J. R. Petta, S. Tarucha, and L. M. K. Vandersypen, Rev. Mod. Phys. **79**, 1217 (2007).

[6] A. V. Khaetskii, D. Loss, and L. Glazman, Phys. Rev. Lett. **88**, 186802 (2002).

[7] I. A. Merkulov, A. L. Efros, and M. Rosen, Phys. Rev. B **65**, 205309 (2002).

[8] F. H. L. Koppens, J. A. Folk, J. M. Elzerman, R. Hanson, L. H. Willems van Beveren, I. T. Vink, H. P. Tranitz, W. Wegscheider, L. P. Kouwenhoven, and L. M. K. Vandersypen, Science **309**, 1346 (2005).

[9] J. R. Petta, A. C. Johnson, J. M. Taylor, E. A. Laird, A. Yacoby, M. D. Lukin, C. M. Marcus, M. P. Hanson, and A. C. Gossard, Science **309**, 2180 (2005).

[10] W. A. Coish and D. Loss, Phys. Rev. B **70**, 195340 (2004).

[11] D. Klauser, W. A. Coish, and D. Loss, Phys. Rev. B **73**, 205302 (2006).

[12] D. Stepanenko, G. Burkard, G. Giedke, and A. Imamoglu, Phys. Rev. Lett. **96**, 136401 (2006).

[13] J. R. Petta, J. M. Taylor, A. C. Johnson, A. Yacoby, M. D. Lukin, C. M. Marcus, M. P. Hanson, and A. C. Gossard, Phys. Rev. Lett. **100**, 067601 (2008).

[14] D. J. Reilly, J. M. Taylor, J. R. Petta, C. M. Marcus, M. P. Hanson, and A. C. Gossard, Science **321**, 817 (2008).

[15] E. A. Laird, J. R. Petta, A. C. Johnson, C. M. Marcus, A. Yacoby, M. P. Hanson, and A. C. Gossard, Phys. Rev. Lett. **97**, 056801 (2006).

[16] W. A. Coish and D. Loss, Phys. Rev. B **72**, 125337 (2005).

[17] J. Särkkä and A. Harju, Phys. Rev. B **77**, 245315 (2008).