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Decoherence and fidelity of single-electron spin states in quantum dots: effects of nuclear hyperfine coupling and double occupancy

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Abstract

The decoherence and fidelity of spin states in a localized single-electron quantum dot in the presence of a dc magnetic field, arising either from the nuclear hyperfine interaction within the dot or due to its coupling with another localized quantum dot, are examined in detail. A general framework for determining the time evolution of the reduced density matrix ρ for a single dot is presented, which is exact up to the second order in interaction with any reservoir. In particular, it is applied to the problem of nuclear hyperfine coupling, and approximate estimates of coherence decay time are made when the nuclear spins are either polarized or unpolarized and the internal dynamics of nuclear spins is determined mainly by the nuclear magnetic dipole–dipole interaction. The fidelity of a pure unperturbed electronic one-qubit spin state is obtained as a function of time, which is exact even on a very short timescale of logic gate operations. The time variation of the fidelity of the same one-qubit state on the localized dot as a part of the direct product with another one-qubit state on another localized dot arising because of coupling between these quantum dots is also calculated in this paper. In this case, we include both the single-particle tunnelling between the dots as well as the direct and exchange Coulomb interactions, including on-site Coulomb repulsion. This allows for the double occupation of a single dot. It is found that the loss of fidelity of such two-qubit states due to double occupancy and additional phase errors in the presence of appreciable dot–dot coupling can become a more severe limiting factor than that due to the hyperfine interaction in individual dots.

1. Introduction

In recent years, there has been a great interest in understanding the nature of coherence decay and relative phase errors of a general spin state in single-electron quantum dots in

semiconductors [1, 2]. This is extremely important because of the possible use of such spin states as a qubit in quantum information processing and computing [3]. For such applications, one has to minimize the coherence decay rate, as far as possible, and find suitable procedures to correct errors in processing due to decay and additional relative phase change of coherently superposed quantum states. Various possible mechanisms for decoherence have been considered in the literature, including spin–orbit coupling, nuclear hyperfine interaction, and coupling to a nearby quantum dot [4–11]. Unless the material has large spin–orbit interaction, at low enough temperatures the dominant mechanisms for decay and additional phase error in spin states are expected to arise from the hyperfine coupling of the electron spin with nuclear spins and from its coupling to a nearby quantum dot. In order to implement any two-qubit or higher qubit logic operations, it is necessary to have a system of two coupled localized single-spin quantum dots in most of the proposals involving the use of quantum dots for quantum computing.

In this paper, we would like to explore the possible hurdles in implementing one-qubit and two-qubit logic operations through single and coupled double localized quantum dots. While processing any general one-qubit spin state $|\Psi(t = 0)\rangle = \alpha(0)|\uparrow\rangle + \beta(0)|\downarrow\rangle$, with the energy difference $\hbar\omega_a$ between the two levels and $|\alpha|^2 + |\beta|^2 = 1$, in the presence of various interactions with the environment, both the change in the relative phase of the coefficients as a function of time t, i.e., the phase of the off-diagonal element of the Hermitian reduced spin-density matrix, and their actual decay, compared to the case of free precession, are important parameters. The combined effect is best described by the fidelity $F(t)$ in the quantum computing language. As defined by Nielsen and Chuang [11], $F(t) = [\langle\Psi(t)|\rho(t)|\Psi(t)\rangle]^{1/2}$, where $\rho(t)$ is the reduced density matrix of the spin system in the presence of interactions with the environment. In the absence of these interactions, the fidelity is 1 (the maximum value possible). Any departure of fidelity F from 1, because of the interactions, determines the performance and the number of logic operations possible. The nature of the departure of fidelity from 1 determines whether it is feasible to find corresponding error correction codes, including phase error corrections. The fidelity can depart very much from 1 even if there is no actual decay or the decay is too slow. The decay timescale for the off-diagonal matrix elements is characterized by the time in which their absolute value changes by a factor $1/e$, whereas the additional phase-error timescale can be characterized by the time in which phase errors change by π. The same situation will occur in processing two-qubit states in a coupled double quantum dot system, which will now have an additional loss of fidelity due to the possibility of double occupancy (both the spins on the same site) and additional phase errors due to single-particle tunnelling and other interactions between the dots.

In what follows, we first investigate the nature of decoherence and fidelity of single quantum dot qubit states, arising from the time variation of the off-diagonal elements of the reduced 2×2 density matrix of the electronic spin-1/2 system in a dc magnetic field, because of the nuclear hyperfine interaction, with N effective nuclear spins within the envelope of the one-electron wavefunction in the localized dot. This is presented in section 2. A typical effective value of N is of the order of 10^5 in a localized dot of the size of 20 nm. To be specific, in this paper we will use all parameters relevant to GaAs single-electronic quantum dots of size 20 nm, with nuclear spin $I = 3/2$ [1]. To obtain the equation governing the time-dependence of the reduced density matrix ρ of the system, we follow the second-order perturbation approach of Bloch and Wangsness [12], but instead of making the Markovian approximation used by them for correlation functions of the surroundings we first present a theory of relaxation decay and time-dependent phase error without the very short correlation time approximation. Estimates of the resulting decay time and relative phase error in the off-diagonal elements of the reduced density matrix are obtained and discussed in the same section.

It will be shown how the relative phase error due to spread in free precession frequency, which gives rise to the well known inhomogeneous line width and decay on ensemble averaging over all possible nuclear spin orientations [9] for unpolarized nuclei, with the timescale of 5 ns in the GaAs dot, can be corrected after each logic operation being performed on the timescale of, say, 0.1 ns. In general, the homogeneous broadening decay time, which determines the number of single logic operations possible, arising from the internal nuclear dynamics involving mainly the nuclear magnetic dipole–dipole interaction with a timescale of 10^{-4} s, depends on the initial spin polarization of the nuclear spins in the dot, and can be quite slow for appreciable nuclear polarizations [11]. The same thing is true for the inhomogeneous phase error or the corresponding decay. A very general spin bath model for environment interacting with a central spin-half system has also been considered by Prokof'ev and Stamp [13]. We will discuss that work in the context of our straightforward approach and final results.

In section 3, we take up the problem of fidelity and decoherence of spin states of a quantum dot when it is coupled to another dot. We explicitly obtain the general solution of the time-dependent Schrodinger equation for two electronic spins localized in quantum dots a and b, respectively, in the presence of an external dc magnetic field, single-particle tunnelling between the dots and effective Coulomb interaction between the electrons. The nature of decay and relative phase errors due to nuclear hyperfine coupling will be same for each individual dot states, as calculated in section 2. For an initial qubit state of the spin localized in dot a, as considered in section 2, and the electronic spin state of dot b being either up or down, we find it enough here to calculate the additional change in the fidelity of such a two-qubit spin state at any time t because of the dot–dot coupling only. This includes the effect of double occupancy, i.e., two spins at the same site [10]. We discuss how difficult it is to overcome the effect of double occupancy and correct for the phase error in this case, to increase the fidelity. One can, of course, increase the distance between the dots from its typical value of 40 nm to decrease the dot–dot coupling parameters, but then the two-qubit logic gate operation times will become too slow and the phase error has still to be corrected before each operation. We conclude our discussion in section 4, which includes suggestions for future experiments on such isolated systems.

2. Effect of hyperfine coupling in a single dot: general theory of relaxation and decoherence

Let us first consider the case of a single quantum dot 'a' represented by one effective spin-1/2 electron localized in the quantum dot and interacting with N_0 nuclear spins in the dot through the familiar contact hyperfine interaction. In the presence of a dc magnetic field B in the z-direction, the total Hamiltonian for the dot can be written as (in units with $\hbar = 1$)

$$H = H_a + H_N + H_{aN} \tag{2.1}$$

$$H_a = \omega_a S_{az}, \qquad \omega_a \equiv \omega_{\mathrm{B}} = g_a \mu_{\mathrm{B}} B \tag{2.2a}$$

$$H_N = -\omega_N \sum_{j=1}^{N_0} I_j^{(0)} + H_N^{(0)} \tag{2.2b}$$

$$H_{aN} = \sum_{j=1}^{N_0} A_j \vec{I}_j \cdot \vec{S}_a \equiv \sum_{q=-1}^{+1} F^{(q)} S^{(-q)} = \sum_{q=-1}^{+1} F^{(-q)} S^{(q)} \tag{2.2c}$$

$$F^{(0)} = \sum_{j=1}^{N_0} F_j^{(0)} = \sum_{j=1}^{N_0} A_j I_j^{(0)}; \qquad F^{(\pm 1)} = \sum_{j=1}^{N_0} F_j^{(\pm 1)} = \sum_{j=1}^{N_0} \frac{A_j}{2} I_j^{(\pm 1)} \tag{2.3}$$

$$I_j^{(0)} = I_{jz}, I_j^{(\pm 1)} = I_{jx} \pm \mathrm{i} I_{jy}; \qquad S^{(0)} = S_{az}, S^{(\pm 1)} = S_{ax} \pm \mathrm{i} S_{ay}. \tag{2.4}$$

In the above expressions, $\vec{I}_j$ represents the jth nuclear spin with magnetic moment $g_N \mu_N \vec{I}_j$, $H_N^{(0)}$ is the nuclear Hamiltonian describing the internal motion of the nuclei, all with the same spin value I, $\vec{S}_a$ represents the electronic spin with magnetic moment $-g_a \mu_B \vec{S}_a$, and H_{aN} is the contact hyperfine interaction of the spin $-1/2$ electron with N_0 nuclear spins. The hyperfine coupling strength $A_j = A v_0 |\Psi(\vec{R}_{aj})|^2$, where v_0 is the effective volume per nuclear spin in the dot and $|\Psi(\vec{R}_{aj})|$ is the amplitude of the electronic wavefunction at the jth nuclear site. For GaAs, $A = \sum_j A_j \equiv N A_1 \approx 10^{11}\ \mathrm{s}^{-1}$ [1], where A_1 is the strength of the hyperfine coupling with the nucleus at the centre of the envelope function. This relation between A and A_1 defines what we call the effective number of nuclei, N.

In the absence of hyperfine interaction, we have

$$\rho_a^{(0)}(t) = A(t) \rho_a^{(0)} A^{-1}(t), \qquad \rho_N^{(0)}(t) = B(t) \rho_N^{(0)} B^{-1}(t), \tag{2.5}$$

where the operators $A(t)$ (not to be confused with the total hyperfine coupling A) and $B(t)$ are given by

$$A(t) = \exp -(\mathrm{i} H_a t), \qquad B(t) = \exp -(\mathrm{i} H_N t) \tag{2.6}$$

and where the commutator $[B(t), A(t)] = 0$. The density matrix of the total system ρ_{aN} satisfies the equation

$$\frac{\mathrm{d}\rho_{aN}}{\mathrm{d}t} = -\mathrm{i}\,[H_a + H_N + H_{aN}, \rho_{aN}]\,. \tag{2.7}$$

Let us assume that, at time $t = 0$, one has

$$\rho_{aN}(t = 0) = \rho_a(0) \rho_N(0) = \rho_a^{(0)} \rho_N^{(0)}, \tag{2.8}$$

where as usual we have the normalization condition

$$\mathrm{Tr} \rho_{aN}(t) = \mathrm{Tr} \rho_a^{(0)}(0) = \mathrm{Tr} \rho_N^{(0)}(0) = 1. \tag{2.9}$$

The reduced density matrix of the electronic system at any time t is defined by

$$\rho(t) = \mathrm{Tr}_N \rho_{aN}(t) = \sum_{f,u} \langle f u |\, \rho_{aN}(t)\, | f u \rangle, \tag{2.10}$$

where $\{|fu\rangle\}$ is the complete set of states of the nuclear reservoir in the absence of the interaction H_{aN},

$$H_N\, |f u\rangle = E_f\, |f u\rangle\,. \tag{2.11}$$

Here, the symbol u labels possible orthogonal degenerate states for a given f with energy E_f. For example, the value of the total z-component of the nuclear spin $M = \sum_j I_{jz} = \sum_j m_{jz}$ will correspond to the label f here. But for a given M, there are many degenerate states possible corresponding to different configurations of the individual values of the nuclear spin states. Thus, in our case, the state $|fu\rangle$ will correspond to the nuclear spin state $|f = M = \sum_j m_{jz}; u = \{m_{jz}\}\rangle$.

The equation for the 2×2 reduced density matrix $\rho(t)$ for the electronic spin system can now be obtained using the familiar interaction picture and the Dyson series expansion up to the second order in the interaction H_{aN}. However, to avoid the first-order terms in H_{aN} in our expansion, it is best to follow the Bloch–Wangsness procedure [12] in which a proper first-order term is added to the system Hamiltonian H_a and subtracted from H_{aN}. This is accomplished by rewriting the Hamiltonian (2.1) as

$$H = \tilde{H}_a + H_N + \tilde{H}_{aN} \tag{2.12}$$

$$\tilde{H}_a = H_a + \delta H, \qquad \tilde{H}_{aN} = H_{aN} - \delta H \tag{2.13a}$$

$$\delta H = \langle H_{aN} \rangle \equiv \mathrm{Tr}_N H_{aN} \rho_N^{(0)} = \sum_f \sum_u \langle fu | H_{aN} | fu \rangle \rho_N^{(0)}(E_f). \tag{2.13b}$$

In the present case, the operator δH in the electronic spin space is

$$\delta H = \left\langle \sum_q F^{(q)} S^{(-q)} \right\rangle = \langle F^{(0)} S^{(0)} \rangle \cong \sum_j A_j (\langle M \rangle / N_0) S^{(0)} = pINA_1 S^{(0)} \tag{2.14}$$

$$\tilde{H}_a = \tilde{\omega}_a S^{(0)}, \qquad \tilde{\omega}_a = \omega_a + \delta\omega_a, \qquad \delta\omega_a \cong pINA_1, \tag{2.15}$$

where $NA_1 = A$ is the total coupling constant of the nuclear spins and p is the degree of initial polarization of the nuclear spins ($-1 \leqslant p \leqslant 1$). The value of $p = 1$ represents complete polarization with each nuclear spin having $m_{Iz} = I$, whereas $p = -1$ corresponds to complete polarization with each $m_{Iz} = -I$. The unpolarized state corresponds to the average $M = 0$, with $p = 0$.

Using the interaction picture, but with free Hamiltonians $\tilde{H}_a$ (equation (2.13*a*)) H_N and interaction $\tilde{H}_{aN}$, and the Dyson series expansion, a straightforward calculation leads to the following general equation for the reduced density matrix to second order in $\tilde{H}_{aN}$:

$$\frac{\mathrm{d}\rho}{\mathrm{d}t} + \mathrm{i}\left[\tilde{H}_a, \rho\right] = -\Gamma(\rho) \tag{2.16}$$

$$\Gamma(\rho) = \int_0^t \mathrm{d}t' L(t, t', \rho(t)) = \int_0^t \mathrm{d}\tau L(-\tau, \rho(t)); \qquad t - t' = \tau \tag{2.17a}$$

$$L(-\tau, \rho(t)) = \sum_q \sum_{q'} \left\{ \begin{array}{c} \Gamma_{qq'}(-\tau) S^{(-q)} S^{(-q')}(-\tau) \rho(t) \\ - \Gamma_{qq'}(-\tau) S^{(-q')}(-\tau) \rho(t) S^{(-q)} \\ + \Gamma_{q'q}(\tau) \rho(t) S^{(-q')}(-\tau) S^{(-q)} \\ - \Gamma_{q'q}(\tau) S^{(-q)} \rho(t) S^{(-q')}(-\tau) \end{array} \right\}, \tag{2.17b}$$

where

$$\Gamma_{qq'}(-\tau) = \langle \tilde{F}^{(q)}(t) \tilde{F}^{(q')}(t') \rangle = \delta_{q',-q} \Gamma_{q,-q}(-\tau) \tag{2.18a}$$

$$\Gamma_{q'q}(\tau) = \langle \tilde{F}^{(q')}(t') \tilde{F}^{(q)}(t) \rangle = \Gamma^*_{q'q}(-\tau) \tag{2.18b}$$

$$\tilde{F}^{(q)} = F^{(q)} - \langle F^{(q)} \rangle; \qquad \tilde{F}^{(q)}(t) = B^{-1}(t) \tilde{F}^{(q)} B(t) \tag{2.18c}$$

$$S^{(q)}(-\tau) = \tilde{A}^{-1}(-\tau) S^{(q)} \tilde{A}(-\tau) = \exp(-\mathrm{i}q\tilde{\omega}_a \tau) S^{(q)}. \tag{2.18d}$$

Here, we have used the fact that the operators $\tilde{F}^{(q)}$ transform as the components of a vector, i.e. like the components $I^{(q)}$ of the total nuclear spin angular momentum; $\tilde{F}^{(-q)}$ is the Hermitian conjugate of $\tilde{F}^{(q)}$.

In order to separate the expressions (2.17*b*) into a sum of two terms of the form $g(-\tau)$ times a Hermitian operator plus $\mathrm{i}h(-\tau)$ times an antiHermitian operator, where g and h are real functions of $-\tau$, let us introduce the following two functions,

$$K^{(1)}_{qq'}(-\tau) = \tfrac{1}{2}(\Gamma_{qq'}(-\tau) + \Gamma_{q'q}(\tau)) = K^{(1)}_q(-\tau)\delta_{q',-q} \tag{2.19}$$

$$K^{(2)}_{qq'}(-\tau) = -\tfrac{1}{2}(\Gamma_{qq'}(-\tau) - \Gamma_{q'q}(\tau)) = K^{(2)}_q(-\tau)\delta_{q',-q} \tag{2.20}$$

with the properties

$$K^{(1)}_{-q}(-\tau) = K^{(1)*}_{q}(-\tau) = K^{(1)}_{q}(\tau) \tag{2.21a}$$

$$K^{(2)}_{-q}(-\tau) = -K^{(2)*}_{q}(-\tau) = -K^{(2)}_{q}(\tau). \tag{2.21b}$$

After some algebra and using the above symmetries of the correlation functions, we obtain

$$\begin{aligned} L(-\tau, \rho(t)) = & \sum_{q=-1}^{1} (a^{(1)}_{q}(-\tau) + a^{(2)}_{-q}(-\tau)) \\ & \times (S^{(-q)}S^{(q)}\rho(t) + \rho(t)S^{(-q)}S^{(q)} - 2S^{(q)}\rho(t)S^{(-q)}) \\ & + \mathrm{i}\sum_{q=-1}^{1} (c^{(1)}_{q}(-\tau))(S^{(-q)}S^{(q)}\rho(t) + \rho(t)S^{(q)}S^{(-q)}), \end{aligned} \tag{2.22}$$

where

$$a^{(1)}_{-q}(-\tau) = a^{(1)}_{q}(-\tau); \qquad a^{(2)}_{-q}(-\tau) = -a^{(2)}_{q}(-\tau); \qquad c^{(1)}_{-q}(-\tau) = -c^{(1)}_{q}(-\tau), \tag{2.23a}$$

$$a^{(1)}_{0}(-\tau) = k_0(-\tau); \qquad a^{(2)}_{0}(-\tau) = 0; \qquad c^{(1)}_{0}(-\tau) = 0, \tag{2.23b}$$

$$a^{(1)}_{1}(-\tau) = k_1(-\tau)\cos\tilde{\omega}_a\tau + p_1(-\tau)\sin\tilde{\omega}_a\tau; \tag{2.23c}$$

$$a^{(2)}_{1}(-\tau) = k_2(-\tau)\cos\tilde{\omega}_a\tau + p_2(-\tau)\sin\tilde{\omega}_a\tau; \tag{2.23d}$$

$$c^{(1)}_{1}(-\tau) = k_1(-\tau)\sin\tilde{\omega}_a\tau - p_1(-\tau)\cos\tilde{\omega}_a\tau, \tag{2.23e}$$

and where the real functions k_i $(i = 0, 1, 2)$, p_j $(j = 1, 2)$ are given by

$$\begin{aligned} & k_0(-\tau) = K^{(1)}_{0}(-\tau); \qquad k_1(-\tau) + \mathrm{i}p_1(-\tau) = K^{(1)}_{1}(-\tau) \\ & k_2(-\tau) + \mathrm{i}p_2(-\tau) = K^{(2)}_{1}(-\tau). \end{aligned} \tag{2.24}$$

Note that k_i are even functions and p_j are odd functions of their argument.

It should be emphasized here that the above formulation gives the familiar Lindblad form [14] as the first term in $\Gamma(\rho)$, and the second term corresponds to a second-order contribution to the system Hamiltonian which has been already corrected to first order. Thus one finds that the effect of the second-order term is to change the system Hamiltonian (2.15) to

$$\tilde{H}_a = \tilde{\omega}_a S^{(0)} \to (\tilde{\omega}_a + c(t))S^{(0)}, \tag{2.25}$$

where

$$c(t) = -2\int_0^t \mathrm{d}\tau\, c^{(1)}_{1}(-\tau). \tag{2.26}$$

In our case we can show that the functions $k_1/2$ and $p_2/2$ are respectively the real and imaginary parts of the correlation function $\Gamma_{xx} = \Gamma_{yy}$, whereas $p_1/2$ and $-k_2/2$ are respectively the real and imaginary parts of $\Gamma_{yx} = -\Gamma_{xy}$. In some situations the cross correlation functions $\Gamma_{yx} = \Gamma_{xy} = 0$, in which case p_1 and $-k_2$ will be zero. However, in general, this is not the case. We now introduce three real relaxation functions defined by

$$\Gamma_0(t) = \int_0^t \mathrm{d}\tau\, a^{(1)}_{0}(-\tau) \tag{2.27}$$

$$\Gamma_1(t) = \int_0^t \mathrm{d}\tau\, a^{(1)}_{1}(-\tau) \tag{2.28}$$

$$\Gamma_2(t) = \int_0^t \mathrm{d}\tau\, a^{(2)}_{1}(-\tau). \tag{2.29}$$

If the nuclear bath is in thermal equilibrium at temperature T then the structure of the reservoir correlation functions are such that it can be shown that as time t approaches $\to \infty$, $(\Gamma_2(\infty)/\Gamma_1(\infty)) = [\exp(\hbar\tilde{\omega}_a/k_{\rm B}T) - 1]/[\exp(\hbar\tilde{\omega}_a/k_{\rm B}T) + 1]$. This then leads to the expected result that at large times the ratio of the diagonal elements of the density matrix of the spin system approaches the Boltzmann factor.

Equations (2.16), (2.17), (2.22) and (2.26), with the above considerations, then lead to two independent equations for determining the diagonal and the off-diagonal matrix elements of the density matrix. In the representation in which the spin-up state is called 1 and the spin-down state is called 2, the equations determining the diagonal and the off-diagonal matrix elements are

$$\mathrm{d}\rho_{11}/\mathrm{d}t = -\mathrm{d}\rho_{22}/\mathrm{d}t = -4\Gamma_1(t)\rho_{11} + 2((\Gamma_1(t) - \Gamma_2(t)) \tag{2.30a}$$

$$\mathrm{d}\rho_{12}/\mathrm{d}t = \mathrm{d}\rho_{21}^*/\mathrm{d}t = -\left(\Gamma_0(t) + 2\Gamma_1(t)\right)\rho_{12} - \mathrm{i}\left(\tilde{\omega}_a + c(t)\right)\rho_{12}. \tag{2.30b}$$

We thus obtain the complete temporal development of ρ_{12} as

$$\rho_{12}(t) = \rho_{12}(0)\exp(-\mathrm{i}\left(\omega_a + \delta\omega_a\right)t)\exp\left(-\mathrm{i}\int_0^t \mathrm{d}t' c(t')\right) \times \exp\left(-\int_0^t \mathrm{d}t'\left(\Gamma_0(t') + 2\Gamma_1(t')\right)\right). \tag{2.31}$$

Until now, our approach has been quite general, with a straightforward derivation of the final result which is exact to the second order in the electron–nuclear coupling. Such a compact form for the final equations determining the complete temporal behaviour of the reduced density matrix is usually not found in the literature. In fact, this form is applicable to any type of coupling between a reservoir and a two-level system with the obvious modification in the form of the interaction and reservoir correlation functions. Further progress in our case can, however, be made only if we know the nuclear correlation functions. Depending upon the initial state of the nuclear spins, these correlation functions depend on the effective number N of the nuclear spins, magnetic field B, the polarization factor p and some correlation timescale $\tau_{c\mu}$ arising from the internal nuclear spin dynamics. This actually requires detailed numerical calculations [1, 15] for the correlation functions. However, one may be able to get a rough estimate of the magnitude of the coherence time if we make certain simplifying assumptions. When the average value of the z-component of spin per nucleus is described by pI which is related to $\langle M\rangle = \langle\sum_j m_{jz}\rangle$, and the total hyperfine coupling constant is replaced by $A = NA_1$, it can be shown that $k_0(-\tau) \to 0$. Similarly, it is possible to neglect $p_1(-\tau)$, at least for vanishing Zeeman splitting of the nuclear spin states compared to electronic Zeeman splitting and small polarization factor. Further, if we assume that, because of the internal dynamics of the nuclear system,

$$k_1(-\tau) \cong \langle|F^{(+1)}|^2\rangle \mathrm{e}^{-|\tau|/\tau_c}; \qquad \langle|F^{(+1)}|^2\rangle \equiv \langle F^{(+1)}F^{(-1)}\rangle, \tag{2.32}$$

the temporal development of ρ_{12} is determined by the function

$$2\Gamma_1(t) = 2\langle\langle|F^{(+1)}|^2\rangle\rangle\int_0^t \mathrm{d}t'\mathrm{e}^{-t'/\tau_c}\cos\tilde{\omega}_a t' = \frac{1}{\tilde{\omega}_a(1+\Omega_c^2)}\left\{\mathrm{e}^{-t'/\tau_c}(\Omega_c^2\sin\tilde{\omega}_a t - \Omega_c\cos\tilde{\omega}_a t) + \Omega_c\right\}, \tag{2.33}$$

where $\Omega_c = \tilde{\omega}_a\tau_c$.

This function has both damped oscillatory terms and a term constant in time. Its precise behaviour depends on Ω_c and $\tilde{\omega}_a t$. The short-time behaviour is complicated. However, only the constant term determines its long-time behaviour

$$2\Gamma_1(t) \to \frac{1}{T_{2h}} = 2\langle|F^{(+1)}|^2\rangle\frac{\tau_c}{1+\Omega_c^2}. \tag{2.34}$$

Similarly, the long-time behaviour of the second-order frequency shift is given by

$$c(t\to\infty) = -2\int_0^{t\to\infty}\langle|F^{(+1)}|^2\rangle \mathrm{e}^{-t/\tau_c}\sin\tilde{\omega}_a t \to -2[\langle|F^{(+1)}|^2\rangle/\tilde{\omega}_a]\frac{\Omega_c^2}{(1+\Omega_c^2)}. \tag{2.35}$$

For the two limiting cases, one can define a homogeneous broadening decay time T_{2h} for the decay of off-diagonal elements of the matrix element and the second-order frequency shift $c(\infty)$, which are given by

$$T_{2h}^{-1} = 2\langle|F^{(+1)}|^2\rangle\tau_c, \qquad c(\infty) = -2\langle|F^{(+1)}|^2\rangle\tilde{\omega}_a\tau_c^2; \qquad \Omega_c \ll 1, \tag{2.36a}$$

and

$$\frac{1}{T_{2h}} = 2\langle|F^{(+1)}|^2\rangle\frac{1}{\tilde{\omega}_a^2\tau_c}, \qquad c(\infty) = -2\langle|F^{(+1)}|^2\rangle/\tilde{\omega}_a; \qquad \Omega_c \gg 1. \tag{2.36b}$$

For GaAs, one can take $\langle|F^{(+1)}|^2\rangle \approx 5\times10^{20}$ s^{-2} and the correlation time for the internal nuclear spin dynamics arising from magnetic dipole interaction to be of the order $\tau_c \approx 10^{-4}$ s. Here $\tilde{\omega}_a = \omega_a + A_1 NIp$ in which $\omega_a = \omega_B \cong 5\times10^{10}$ s^{-1} for a typical 2 T magnetic field. This implies that Ω_c is always much greater than 1, and one has to use the estimate given by equation (2.36*b*) for the homogeneous broadening decay time T_{2h}. In the unpolarized state, $p = 0$, we find $T_{2h} \approx 2\times10^{-4}$ s. However, when $p \neq 0$, T_{2h} is increased further. For $\Delta\omega_a = A_1 NIp \gg \omega_a$, $T_{2h} \approx (p^2 N\tau_c)/2$ since $\langle|F^{(+1)}|^2\rangle$ is proportional to N. In such a case, even for $p \cong 10^{-1}$, $N = 10^5$, T_{2h} becomes of the order 5×10^{-2} s. Of course, in that case the spin–orbit interaction will become the dominant mechanism for coherence decay with relaxation times in the range of 10^{-3} s.

We must emphasize here that the above estimates of decay of the off-diagonal element only refer to the long-time behaviour of the integral of the function $\Gamma_1(t)$. There is the additional relative phase error arising from the change in the precision frequency due to the presence $\delta\omega_a$ and $c(t)$ in equation (2.31). Note that in the case of unpolarized nuclei, when $\delta\omega_a = 0$, $c(\infty)$ is still finite even if the internal nuclear dipolar correlation time $\tau_c \to \infty$, as can be seen from equation (2.36*b*). The limiting expression is consistent with the usual time-independent second-order energy shift calculation giving rise to an additional relative phase. Normally, for $p = 0$, one averages this inhomogeneous spread in the precession frequency of the electronic spin over an ensemble (thermal or otherwise) of dots with different nuclear orientations with a phenomenological Gaussian distribution [9] of the precession frequencies with a width $[\langle(\Delta\omega)^2\rangle]^{1/2} = [(16/3)\langle|F^{(+1)}|^2\rangle/N]^{1/2} \approx 2\times10^8$ s^{-1}, in our notation. This phenomenological averaging leads to the familiar inhomogeneous line broadening and a temporal decay of the off-diagonal elements of the form, $\langle\exp(\mathrm{i}\omega t)\rangle = \langle\cos\omega t\rangle = \exp(-\langle(\Delta\omega)^2\rangle t^2/2)$ [9]. In fact if one averages $\exp(\mathrm{i}\omega t)$ over any symmetric distribution for ω which satisfies the central limit relations between their even moments, which are the same as in the case of the Gaussian distribution, we will always get such a decay and inhomogeneous broadening. If we average the long-time form of the phase variation $\exp(-\mathrm{i}c(\infty)t)$ in our exact solution (2.31), we will get the same type of additional decay due to inhomogeneous broadening with the decay time of the order of 5 ns. This spreading of precession frequency is, however, a reversible process, and can be corrected by using the well known method of the pulsed spin-echo technique [1, 16]. In our case, each of the one-qubit logic operations

is supposed to be done at a very fast rate on the timescale of $\Delta t_{\rm op} \approx 10^{-10}$ s per operation. For such a situation, no averaging of the phase error factor is possible, but the net phase error has still to be corrected before each logic operation using the spin-echo technique or other techniques for correcting such phase errors. During the single logic operation in time $\Delta t_{\rm op}$ at time t, the off-diagonal matrix element will change by a phase $c(t)\ \Delta t_{\rm op}$, in addition to a slower decay determined by the scale of T_{2h}. Whereas the homogeneous decay is irreversible and it ultimately determines how many single logic operations are possible during T_{2h}, the reversible phase error of the single qubit due to the inhomogeneous frequency spread can be corrected before each logic operation. The time between two logic operations can be 0.5 ns. The phase error timescale, the time for it to change by π, is still of the order of 5 ns. But note also that the actual temporal variation of the phase error factor in equation (2.31) is quite complicated compared to its usual long-time behaviour used in most such phenomenological averaging [9, 13]. Prokof'ev and Stamp [13] have developed a very general model for the dynamics of a central effective two-level system, equivalent to our spin-half system, in the presence of its general coupling to a spin bath (reservoir). It is not restricted to the case of the nuclear hyperfine coupling of a spin-half electron. Although they do mention this problem, the actual physical applications discussed there in detail do not include this problem. They also consider the effect of an external magnetic field, but that is not the main focus of the work. The main focus there is to explain different types of phenomenological averaging and apply these results to different physical problems in weak external magnetic fields. Our approach is to treat the problem of the hyperfine coupling, in the presence of a dc magnetic field, using a microscopic theoretical approach for obtaining the detailed temporal evolution of the reduced density matrix of the central spin which is exact to the second order in coupling even for short times.

Let us now calculate the fidelity F of a pure initial state $|\chi\rangle$ of the system with respect to the general reduced density matrix $\rho(t)$ obtained in the presence of the hyperfine coupling. It is defined by

$$F = [\langle\chi|\,\rho\,|\chi\rangle]^{1/2}. \tag{2.37}$$

In the absence of hyperfine coupling, a typical superposed qubit state $\frac{1}{\sqrt{2}}(|\uparrow_a\rangle + |\downarrow_a\rangle)$ develops in time as

$$|\chi(t)\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow_a\rangle e^{-i\omega_a t/2} + |\downarrow_a\rangle e^{i\omega_a t/2}\right). \tag{2.38}$$

The fidelity of this state with respect to the ρ considered here in the presence of hyperfine coupling is

$$F(t) = \frac{1}{\sqrt{2}}\left[1 + 2\,{\rm Re}\left(\rho_{12}(t)e^{i\omega_a t}\right)\right]^{1/2}. \tag{2.39}$$

If we use equation (2.31) for $\rho_{12}(t)$, with $\rho_{12}(0) = e^{-i\omega_a t/2}$, $\omega_{\rm B} = \omega_a$, corresponding to the non-interacting state, we obtain

$$F(t) = \frac{1}{\sqrt{2}}\left[1 + \left(\cos\left(\delta\omega_a t + \delta_2(t)\right)\ e^{-\gamma(t)}\right)\right]^{1/2}, \tag{2.40}$$

where the general non-exponential damping factor $\gamma(t)$ is given by

$$\gamma(t) = \int_0^t dt'\left[\Gamma_0\left(t'\right) + 2\Gamma_1\left(t'\right)\right] \tag{2.41}$$

and $\delta_2(t)$ is given by

$$\delta_2(t) = \int_0^t dt' c(t'). \tag{2.42}$$

In the absence of interactions $F(t)$ goes to 1, as expected. The complicated oscillations in the above expression come from the energy shifts $\delta\omega_a$ and $\delta_2(t)$. For unpolarized nuclei $\delta\omega_a = 0$, and $\delta_2(t)$ represents the second-order phase error which has to be corrected before each logic gate operation (to be performed at the rate of, say, 0.1 ns, at intervals of, say, 0.5 ns) in quantum processing.

3. Effect of coupling to another localized quantum dot

In this section, we will consider the possibility of coherence decay, phase error and the loss of fidelity of spin states of the quantum dot 'a' due to its coupling with another spin localized at a second quantum dot 'b'. We now deal with two effective single-electron quantum dots interacting via the Coulomb interaction between the electrons with the possibility of single-particle tunnelling between them. The effect of the Coulomb interaction is here parameterized in terms of the integrals involving the Coulomb interaction in first order. Since the coherence decay and relative phase error due to nuclear hyperfine coupling in each individual dots can be obtained from our treatment of the hyperfine coupling in the previous section, here it is enough for us to calculate the additional effect which arises from the dot–dot coupling. For any two-qubit logic operation one cannot avoid this coupling.

In the absence of Coulomb interaction and tunnelling, let us denote the single-particle states localized at 'a' and 'b', respectively, by

$$|a\sigma\rangle \equiv |w_a(\vec{r})\chi_{a\sigma}\rangle, \qquad |b\sigma\rangle \equiv |w_b(\vec{r})\chi_{b\sigma}\rangle, \qquad \sigma = \uparrow, \downarrow \tag{3.1}$$

where $w_a(\vec{r})$ refers to the space part and $\chi_{a\sigma}$ the spin part of the electron wavefunction for the quantum dot 'a', with similar meaning for $w_b(\vec{r})$ and $\chi_{b\sigma}$. One then has the following six two-particle states for the combined system:

$$|u_1\rangle = |a\uparrow, b\downarrow\rangle \equiv c^+_{a\uparrow}c^+_{b\downarrow}|0\rangle; \qquad |u_2\rangle = |a\downarrow, b\uparrow\rangle \equiv c^+_{a\downarrow}c^+_{b\uparrow}|0\rangle \tag{3.2a}$$

$$|u_3\rangle = |a\uparrow a\downarrow, 0\rangle \equiv c^+_{a\uparrow}c^+_{a\downarrow}|0\rangle; \qquad |u_4\rangle = |0, b\uparrow b\downarrow\rangle \equiv c^+_{b\uparrow}c^+_{b\downarrow}|0\rangle \tag{3.2b}$$

$$|u_5\rangle = |a\uparrow, b\uparrow\rangle \equiv c^+_{a\uparrow}c^+_{b\uparrow}|0\rangle; \qquad |u_6\rangle = |a\downarrow, b\downarrow\rangle \equiv c^+_{a\downarrow}c^+_{b\downarrow}|0\rangle. \tag{3.2c}$$

It is convenient to use the spin singlet and triplet combinations of $|u_1\rangle, |u_2\rangle$ along with symmetric and antisymmetric combinations of double-occupancy states $|u_3\rangle, |u_4\rangle$:

$$\text{Triplet: } |v_5\rangle = |u_5\rangle, \qquad |v_6\rangle = |u_6\rangle, \qquad |v_1\rangle = \frac{1}{\sqrt{2}}(|u_1\rangle + |u_2\rangle) \tag{3.3a}$$

$$\text{Singlet: } |v_1\rangle = \frac{1}{\sqrt{2}}(|u_1\rangle - |u_2\rangle) \tag{3.3b}$$

$$\text{Double occupancy : } |v_3\rangle = \frac{1}{\sqrt{2}}(|u_3\rangle + |u_4\rangle), \qquad |v_4\rangle = \frac{1}{\sqrt{2}}(|u_3\rangle - |u_4\rangle). \tag{3.3c}$$

The effective Hamiltonian for the coupled dots can be written in the form

$$H = H_a + H_b + H_{ab}, \tag{3.4}$$

where

$$H_a = \omega_a S_{az} + \sum_\sigma \varepsilon_a c^+_{a\sigma}c_{a\sigma} \tag{3.5a}$$

$$H_b = \omega_b S_{bz} + \sum_\sigma \varepsilon_b c^+_{b\sigma}c_{b\sigma} \tag{3.5b}$$

$$H_{ab} = (K+J)|v_2\rangle\langle v_2| + (K-J)(|v_1\rangle\langle v_1| + |v_5\rangle\langle v_5| + |v_6\rangle\langle v_6|) + \tfrac{1}{2}(U_a + U_b)(|v_3\rangle\langle v_3| + |v_4\rangle\langle v_4|)$$

$$+ \tfrac{1}{2}(U_a - U_b)(|v_3\rangle\langle v_4| + |v_4\rangle\langle v_3|)$$
$$+ \frac{t_{ab}}{2}(c^+_{a\uparrow}c_{b\uparrow} + c^+_{b\uparrow}c_{a\uparrow} + c^+_{a\downarrow}c_{b\downarrow} + c^+_{b\downarrow}c_{a\downarrow}). \tag{3.5c}$$

In the above equations the parameters ε_a and ε_b refer to the energy of one electron in the dots 'a' and 'b' respectively, and the tunnelling energy t_{ab} refers to the case when only one electron is present in the two dots. The effect of Coulomb interaction when two electrons are present in the system is taken into account through the parameters K, J, U_a, U_b. Here K is the direct Coulomb integral, $\langle w_a(1)w_b(2)|V_c(1,2)|w_a(1)w_b(2)\rangle$, between two electrons, one in 'a' and the other in 'b', J is the corresponding exchange integral $\langle w_a(1)w_b(2)|V_c(1,2)|w_b(1)w_a(2)\rangle$, and $U_{a,b}$ are the on-site repulsion energies with $U_a = \langle w_a(1)w_a(2)|V_c(1,2)|w_a(1)w_a(2)\rangle$ (and a similar expression for U_b). $V_c(1,2)$ is the Coulomb interaction between two electrons.

We first note that $|v_5\rangle, |v_6\rangle$ are eigenstates of the total Hamiltonian:

$$H|v_5\rangle = \{\varepsilon_a + \varepsilon_b + (\omega_a + \omega_b)/2 + (K - J)\}|v_5\rangle \tag{3.6}$$
$$H|v_6\rangle = \{\varepsilon_a + \varepsilon_b - (\omega_a + \omega_b)/2 + (K - J)\}|v_6\rangle. \tag{3.7}$$

The remaining four states are coupled and the corresponding Hamiltonian matrix in this 4×4 subspace is given by

$$H = \begin{pmatrix} E_1 & \omega_{ab} & 0 & 0 \\ \omega_{ab} & E_2 & t_{ab} & 0 \\ 0 & t_{ab} & E_3 & \Omega_{ab} \\ 0 & 0 & \Omega_{ab} & E_3 \end{pmatrix} \tag{3.8a}$$

where we have introduced the following notations:

$$\begin{aligned} &E_1 = \varepsilon_a + \varepsilon_b + K - J; \qquad E_2 = \varepsilon_a + \varepsilon_b + K + J; \\ &E_3 = \varepsilon_a + \varepsilon_b + \frac{U_a + U_b}{2}; \qquad \omega_{ab} = \frac{\omega_a - \omega_b}{2}; \\ &\Omega_{ab} = \varepsilon_a - \varepsilon_b + \frac{U_a - U_b}{2}. \end{aligned} \tag{3.8b}$$

For identical dots, $\varepsilon_a = \varepsilon_b = \varepsilon$, $\omega_a = \omega_b = \omega$, $U_a = U_b = U$, and by choosing the origin of the energy scale to be $2\varepsilon = 0$, this matrix reduces to

$$H = \begin{pmatrix} K - J & 0 & 0 & 0 \\ 0 & K + J & t_{ab} & 0 \\ 0 & t_{ab} & U & 0 \\ 0 & 0 & 0 & U \end{pmatrix}. \tag{3.9}$$

From this we see that $|v_1\rangle, |v_4\rangle$ are eigenstates with eigenvalues $(K - J), U$ respectively and the states $|v_2\rangle, |v_3\rangle$ are coupled. We may then write the complete set of eigenvectors and their corresponding eigenvalues in the form

$$H|\Phi_i\rangle = \omega_i|\Phi_i\rangle, \qquad i = 1, \ldots, 6 \tag{3.10}$$
$$|\Phi_1\rangle = |v_1\rangle; \qquad \omega_1 = K - J \tag{3.11}$$
$$|\Phi_4\rangle = |v_4\rangle; \qquad \omega_4 = U \tag{3.12}$$
$$|\Phi_5\rangle = |v_5\rangle; \qquad \omega_5 = \omega_{\mathrm{B}} + K - J \tag{3.13}$$
$$|\Phi_6\rangle = |v_6\rangle; \qquad \omega_6 = -\omega_{\mathrm{B}} + K - J \tag{3.14}$$
$$|\Phi_3\rangle = \frac{|v_2\rangle + C_3|v_3\rangle}{\sqrt{1 + C_3^2}}; \qquad \omega_3 = \frac{U + K + J}{2} + \frac{\Delta}{2} \tag{3.15}$$
$$|\Phi_2\rangle = \frac{|v_3\rangle - C_3|v_2\rangle}{\sqrt{1 + C_3^2}}; \qquad \omega_2 = \frac{U + K + J}{2} - \frac{\Delta}{2} \tag{3.16}$$

where

$$\Delta = \left[(U - K - J)^2 + 4t_{ab}^2\right]^{1/2}, \qquad C_3 = \frac{U - K - J + \Delta}{2t_{ab}}. \tag{3.17}$$

In a practical situation, it is possible to change the barrier properties through external means, by applying a gate voltage between the dots. It is equivalent to changing the distance $d = 2a$ between the dots. This will change t_{ab}, K and J which decrease exponentially with the distance. For arbitrary variations of these quantities with time, it is not possible to find analytic solution of the Schrodinger equation to determine the state of the system $|\Psi(t)\rangle$. However, if these quantities are kept constant during a given time interval, it is straightforward to find $|\Psi(t)\rangle$ at any time during this interval. Assuming this is indeed the case, during this period the state of the system is given by

$$|\Psi(t)\rangle = \sum_{i=1}^{6} d_i \mathrm{e}^{-\mathrm{i}\omega_i t} |\Phi_i\rangle \tag{3.18}$$

in which the coefficients d_i have to be determined from the given initial state at $t = 0$.

Let us assume that the initial state at $t = 0$ is given by the non-interacting state

$$\begin{aligned} |\chi(0)\rangle_{ab} &= \frac{1}{\sqrt{2}}\left[|a\uparrow\rangle + |a\downarrow\rangle\right]|b\downarrow\rangle \\ &= \frac{1}{2}\left(|v_1\rangle + |v_2\rangle\right) + \frac{1}{\sqrt{2}}|v_6\rangle \equiv |\Psi(t=0)\rangle\,. \end{aligned} \tag{3.19}$$

Although our complete solution allows us to compute the fidelity $F(t)$ of any general two-qubit state, which may or may not be entangled, the illustrative specific form chosen above is to see how the dot–dot coupling affects the qubit state of the dot a, considered in section 2 while calculating its fidelity in the presence of hyperfine interaction. We find that the state at time t in the presence of coupling is then given by

$$\begin{aligned} |\Psi(t)\rangle = &\left\{\frac{1}{2}\mathrm{e}^{-\mathrm{i}\omega_1 t}|v_1\rangle + \frac{1}{2\left(1+C_3^2\right)}\left((\mathrm{e}^{-\mathrm{i}\omega_2 t}C_3^2 + \mathrm{e}^{-\mathrm{i}\omega_3 t})\right)|v_2\rangle\right. \\ &\left. + \frac{C_3}{2\left(1+C_3^2\right)}\left(\mathrm{e}^{-\mathrm{i}\omega_3 t} - \mathrm{e}^{-\mathrm{i}\omega_2 t}\right)|v_3\rangle + \frac{1}{\sqrt{2}}\mathrm{e}^{-\mathrm{i}\omega_6 t}|v_6\rangle\right\} \\ = &\sum_i g_i(t)\,|v_i\rangle\,. \end{aligned} \tag{3.20}$$

On the other hand, in the absence of coupling between dots, the coherent spin state $|\Phi\rangle$ would have evolved as

$$|\chi(t)\rangle_{ab} = \left[\frac{1}{2}\left(|v_1\rangle + |v_2\rangle\right) + \frac{1}{\sqrt{2}}\mathrm{e}^{\mathrm{i}\omega_{\mathrm{B}} t}|v_6\rangle\right]. \tag{3.21}$$

The probability $P_{\mathrm{d}}(t)$ for double occupancy at time t is given by the square of the magnitude of the amplitude of the $|v_3\rangle$, i.e., by $|g_3(t)|^2$ in equation (3.20). This term is absent in equation (3.21) and arises only due to the coupling between the dots [10, 17]. Explicitly, one finds

$$\begin{aligned} P_{\mathrm{d}}(t) &= \frac{C_3^2}{\left(1+C_3^2\right)^2}\sin^2\left((\omega_3 - \omega_2)\,t/2\right) \\ &= \frac{t_{ab}^2}{\Delta^2}\sin^2\left(\Delta t/2\right). \end{aligned} \tag{3.22}$$

Although there is no explicit exponential decay of the matrix elements of the density matrix in this problem, one can get an idea about the degree of phase error and the loss of fidelity by calculating $F(t)$ of the non-interacting state $|\chi(t)\rangle_{ab}$. One finds

$$F(t) = [\langle\chi(t)|\rho(t)|\chi(t)\rangle]^{1/2} = |\langle\chi(t)|\Phi(t)\rangle| = \frac{1}{2}\Big[\frac{5}{2} - P_{\rm d}(t) + \frac{3}{2\left(1+C_3^2\right)} \times \left\{C_3^2\cos t\,(K-J-\omega_2) + \cos t\,(K-J-\omega_3)\right\}\Big]^{1/2}, \tag{3.23}$$

in which the relations $K - J = \omega_1 = \omega_6 + \omega_{\rm B}$ have been used. Note that in the absence of coupling or at $t = 0$, the fidelity is 1, as expected. Apart from the two oscillatory terms in equation (3.23) which take both positive and negative values, the fidelity is always reduced if there is double occupancy. The double occupancy probability goes to zero at times $t = T_n$, where

$$|\omega_3 - \omega_2|\,T_n = \Delta T_n = 2n\pi, \qquad n = 1, 2, \ldots. \tag{3.24}$$

For such times, the fidelity is

$$F(T_n) = \tfrac{1}{2}\left[\tfrac{5}{2} + \tfrac{3}{2}\cos T_n\,|K - J - \omega_2|\right]^{1/2}. \tag{3.25}$$

In addition, if it is possible to choose the coupling parameters by adjusting the distance between the dots such that one can have

$$|K - J - \omega_2|\,T_n = 2m\pi, \qquad m = 1, 2, \ldots \tag{3.26}$$

or

$$|K - J - \omega_2|\,T_n = (2m+1)\,\pi, \qquad m = 0, 1, 2, \ldots \tag{3.27}$$

we can get a perfect fidelity of 1 or a perfect swap of states at a and b, respectively. When the conditions (3.24) and (3.26) are simultaneously satisfied, we get a fidelity of 1, with the final state the same as the state (3.21), apart from an overall phase factor $\exp it(K - J)$. On the other hand, if the conditions (3.24) and (3.27) are satisfied at the same time, one has a perfect swap, with the final state.

$$\left|\chi'(t)\right\rangle = \frac{1}{\sqrt{2}}\left[\frac{1}{\sqrt{2}}\left(|v_1\rangle - |v_2\rangle\right) + {\rm e}^{{\rm i}\omega_{\rm B}t}\,|v_6\rangle\right]{\rm e}^{-{\rm i}t(K-J)} = \frac{1}{\sqrt{2}}\left[|a\uparrow, b\uparrow\rangle + {\rm e}^{{\rm i}\omega_{\rm B}t}\,|a\downarrow, b\downarrow\rangle\right]{\rm e}^{-{\rm i}t(K-J)}. \tag{3.28}$$

Note that the minimum time to complete one such two-qubit operation is given by $(K - J - \omega_2)^{-1} \approx -2J + t_{ab}^2/U$. The above conditions can be satisfied only if one can adjust the coupling parameters very precisely. This is a very difficult task in practice. In general one has to live with fidelity less than 1 and an imperfect swap operation.

Before we proceed further, we must give an estimate of the coupling parameters for typical GaAs quantum dots with individual size of 20 nm and distance $d = 2a$ between the two dots of the order of 40 nm. In the absence of an external magnetic field, each effective one-electron GaAs quantum dot, with an effective electron mass of 0.67 m, behaves like a large atom with the new dot Bohr radius $a_{\rm Bd} = 10$ nm in our case. All parameters are scaled in terms of the value of the ratio $a_{\rm Bd}/a_{\rm B} \approx 200$, compared to a usual atom, with an additional reduction of the Coulomb interaction by the dielectric constant of GaAs. The energy scale is scaled down from 1 eV to about 5 meV. A typical value of the onsite Coulomb repulsion energy U is about 0.5 meV, in energy units, in a dot confined in a harmonic potential well of size 20 nm and oscillator energy

$\hbar\omega_0 = 3$ meV. The tunnelling parameter t_{ab}^2/U and Coulomb integrals K and J between electrons fall off approximately as $\exp(-d^2/4a_{\mathrm{Bd}}^2)$, and for chosen parameters, one finds [11], $t_{ab}/U = 0.5$, $t_{ab} \approx 0.25$ meV, $K, J \approx 0.05$ meV $\cong 5 \times 10^{10}$ s^{-1}, $t_{ab}^2/U \approx 10^{11}$ s^{-1}. This implies that $t_{ab}^2/\Delta^2 \approx 0.25$. Equations (3.22) and (3.23) then show that the maximum loss of fidelity due to double occupancy and the phase error can be as high as 57%. The loss due to the double occupancy can of course be reduced considerably by increasing the distance between the dots [11, 18], but that will reduce other coupling parameters to make the two-qubit operation slower than 10^{-10} s per operation. Even then one will require correcting this phase error to avoid the loss of fidelity. The phase error timescale is determined by $(K - J - \omega_2)^{-1}$ which will then increase to say 10^{-9} s. But, unless this phase error is corrected before each operation, this will be a more severe limiting factor than the decay of coherence of individual dot states due to nuclear hyperfine coupling. Note that all these estimates are for fixed dot–dot coupling parameters with no fluctuations. Any fluctuation even at the level of 1% due to inhomogeneity in sample preparation can lead to an additional inhomogeneous decay time of 10^{-7}–10^{-8} s, on averaging, which is not so easy to correct as in the case of a single qubit, discussed in the previous section.

4. Conclusions

In the preceding two sections, we have tried to estimate the coherence decay time, the relative phase error time and the loss of fidelity of a pure superposed one-qubit spin state in a single quantum dot and of a two-qubit state in two coupled single-electron quantum dots. In quantum logic gate operations, both these times are important. When the phase errors or the corresponding inhomogeneous broadening decay can be corrected in certain situations before each logic operation, the irreversible homogeneous decay time of the coherence then really determines the number of logic operations possible within this decay time. For this, in section 2 we presented a general theory of decoherence and relaxation in a spin-1/2 system interacting with a reservoir, making only the second-order perturbation approximation for the coupling to the reservoir. This was applied to the case of decoherence of electronic spin states in a single quantum dot in the presence of a dc magnetic field, due to its interaction with nuclear spins in the dot via the hyperfine contact interaction, which is exact even for short timescales of single logic operation. Using simplifying assumptions regarding the nuclear spin correlation functions, it was estimated that long-time transverse relaxation time T_{2h} due to homogeneous broadening arising from nuclear dipole interaction will be of order 2×10^{-4} s if the nuclear spins are unpolarized. This can be increased considerably if the nuclear spins are polarized. But then the dominant decoherence mechanism may be the spin–orbit interaction in the materials. There is an additional relative phase error due to a second-order inhomogeneous spread of precession frequency of the electronic spin, even for unpolarized nuclei, at a much faster timescale of 5 ns. But this can be corrected before any one-qubit operation which is expected to be performed at the timescale of 0.1 ns at intervals of, say, 0.5 ns. In general, the fidelity is less than 1 and is minimum when the off-diagonal element of the system reduced density matrix finally goes to zero for $t \gg T_{2h}$. It was noted that more realistic estimate of decoherence in this case requires numerical calculation of nuclear spin correlation functions. We propose to take this up in a later work.

We have shown in section 3 that the coupling of two quantum dots because of the electron–electron interaction and single-particle tunnelling leads to double occupancy of sites a and b of the dots and additional phase errors in two-qubit states. This is in addition to the homogeneous decay and phase error of respective states due to hyperfine coupling in each individual dot. Although it is possible in principle to choose times such that double occupancy probability

goes to zero [10] and adjust the dot–dot distance in such a way that fidelity of the two-qubit state can be made 1, this is not an easy task. In general, for nearby dots this becomes a major source for the loss of fidelity.

For the use of quantum dots for efficient quantum processing and computing, one requires to implement both one-qubit as well as two-qubit logic operations at a fast timescale. For this to happen, precise experiments on a single-dot system as well as on a coupled-dot system have to be performed on timescales of 0.1 ns. One has to try to implement and measure the fastest timescale possible for a single-qubit operation (rotation on the Bloch sphere) and the additional phase error during the operation time. One has to see how this phase error acquired between two logic operations can be corrected before each new operation and determine how many such logic operations are possible in time T_{2h}. For the case of two-qubit logic operations using a coupled dot, one has to determine whether the interaction parameters can be precisely controlled to minimize the additional loss of fidelity.

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