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Decay of Rabi oscillations induced by magnetic dipole interactions in dilute paramagnetic solids

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Decay of Rabi oscillations of equivalent spins diluted in diamagnetic solid matrix and coupled by magnetic dipole interactions is theoretically studied. It is shown that these interactions result in random shifts of spin transient nutation frequencies and thus lead to the decay of the transient signal. Averaging over random spatial distribution of spins within the solid and over their spectral positions within magnetic resonance line, we obtain analytical expressions for the decay of Rabi oscillations. The rate of the decay in the case when the half-width of magnetic resonance line exceeds Rabi frequency is found to depend on the intensity of resonant microwave field and on the spin concentration. The results are compared with the literature data for $E_1{}'$ centers in glassy silica and $[AlO_4]^0$ centers in quartz.

Rabi oscillations (or transient nutations) represent transitions between the states of quantum dipole driven by electromagnetic wave of resonant frequency [1]. Early observations of Rabi oscillations (RO) were accomplished on nuclear and electronic magnetic dipoles in NMR [2] and ESR [3] respectively, and on electric dipole moment of an atom in optical resonance [4]. The successful observation of RO in magnetic resonance imposes a number of severe constraints on experimental apparatus: low response time and high sensitivity of radiofrequency circuits, narrow bandwidth and high intensity of the generated electromagnetic field [5]. With the development of magnetic resonance techniques (pulsed NMR and ESR, spin echo) it became possible to observe RO at higher power levels and in a variety of systems, including those with coherence times $< 1\,\mu s$, such as electronic spins in molecular magnets [6]. In magnetic resonance, a comparison of the decay time τ_R of RO and phase relaxation time T_2 reveals how transient nutations driven by resonant microwave (MW) field affect coherence dynamics of the system of spins. Apart from purely academic interest, the answer to this question has an important practical application. In quantum computation, several perspective implementations of a quantum bit (qubit) include electronic or nuclear spin qubits [7] and trapped ion-based optical qubits [8]. They are operable with the application of electromagnetic transient pulses. During a short time interval of the pulse a qubit is in transient regime, i.e. accomplishes RO. If the number of successive operations on the qubit is sufficiently high, one must take into account not only the decoherence induced during time intervals between the pulses, but the one accumulated during RO. In magnetic resonance, the detected RO decay due to various reasons. The principal reasons are (i) static [2] and MW [2, 9, 10] field inhomogeneities, (ii) inhomogeneous broadening of magnetic resonance line [2], (iii) radiation damping [11], (iv) spin-spin and spin-lattice interactions [2]. However, (i) and (ii) lead only to the time-independent distribution of Rabi frequencies of spins in the solid; whereas the total magnetization M of the spin system is damped, the state of a single spin remains coherent. The radiation damping (iii) may be overcome if the detection by means of spin echo sequence is used. Of the abovementioned mechanisms only (iv) result in "true" decoherence, i.e. irreversible change of a single spin state due to its interaction with local environment. Typically, at least at liquid helium temperatures, spin-lattice relaxation times T_1 much exceed phase relaxation times T_2. Consequently, spin-spin interactions are of primary interest in the study of decoherence during the transient regime.

The first description of RO decay was presented in the framework of Bloch model [2]. According to Bloch equations, assuming $T_1 \gg T_2$, the transverse magnetization in transient regime exhibits the damped oscillations of the form [2]:

$$M_\perp(t) \sim \begin{cases} e^{-t/2T_2}\sin(\Omega_R t)\,, & \sigma \ll \Omega_R, \\ e^{-t/2T_2}J_0(\Omega_R t)\,, & \sigma \gg \Omega_R, \end{cases} \tag{1}$$

where Ω_R is Rabi frequency (typically of the order of $0.1\div 10\,\mathrm{MHz}$) proportional to the MW field amplitude, $J_0(x)$ is Bessel function of the first kind, σ is a standard deviation of inhomogeneously broadened resonance line, and we distinguish between two cases of weak ($\sigma \ll \Omega_R$) and strong ($\sigma \gg \Omega_R$) inhomogeneity. The latter case is typical of ESR, where because of crystal lattice imper-

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fections, spatial inhomogeneity of the external magnetic field, exchange, dipolar or hyperfine interactions with magnetic impurities of other species, etc. [11, 12], Larmor precession frequencies are distributed statically in the range up to tens of MHz. The damping rate of RO, according to Bloch model, is equal in both cases and independent of Ω_R : $\tau_R^{-1} = T_2^{-1}/2$.

Probably the first experiments that revealed inadequacy of Bloch equations in transient regime of magnetic resonance were ESR measurements of E_1'-centers in glassy silica [13, 14] and of $[\mathrm{AlO_4}]^0$ centers in quartz [13]. When $\sigma \gg \Omega_R$, the detected RO were found to be of the form $M_\perp \sim e^{-t/\tau_R} J_0(\Omega_R t)$, and the decay rates contained two terms,

$$\tau_R^{-1} = \alpha + \beta \Omega_R, \tag{2}$$

with constant dimensionless coefficient $\beta \sim 10^{-2}$. The peculiar linear dependence of τ_R^{-1} on Ω_R (so-called "anomalous decay" of RO [13]) was in contrast to the predictions of Bloch model (1). Later, the decay rates of the form (2) were obtained for a variety of electronic spin systems, including rare earths [5, 10, 15] and transition metal ions [16, 17]. Up to the moment, the only explanation of the term was given in the framework of modified Bloch equations (MBEs) [18, 19]. In particular, in the semi-phenomenological model of Shakhmuratov et al [18], it is suggested that the driving MW field induces stochastic local magnetic field proportional to the MW field amplitude, and thus the term $\sim \Omega_R$ is included into Bloch equations. Since the measured parameter β was concentration-dependent, the stochastic field was ascribed to spin-spin interactions between paramagnetic ions [14]. However, no estimation of the amplitude of the stochastic field can be given in the framework of phenomenological MBEs [14, 19].

At sufficiently low spin concentrations, the most important spin-spin interactions are long-range magnetic dipole (MD) interactions. Further, we can distinguish between the spins of A and B types [20, 21]. The first, A, have Larmor frequencies close to resonance and thus are driven by the resonant transient pulse. The second group, B, contains spins with precession frequencies far from resonance. RO decay of a single A spin interacting with the bath of B spins was considered in [22]. An example of such a system is a single electronic spin coupled to a bath of nuclear spins [23]. Completely different dynamics has the system of only A spins. There the transient signal is recorded not only from a single spin but from a great number of equivalent spins interacting with each other. While in [22] internal bath dynamics was represented via random field with phenomenological correlation function, we present here a detailed *ab initio* calculation of dynamics of A spin bath in transient regime.

Let us consider a diamagnetic solid matrix containing a small concentration of paramagnetic centers. In the common case when the ground state of a center is the isolated doublet, one introduces (pseudo-)spin $S = 1/2$. For simplicity, we accept also that the interaction of j-th center with the external magnetic field is represented via almost isotropic tensor: $g^j_{\alpha\beta} \approx g_e \delta_{\alpha\beta}$. All the subsequent calculations can be easily generalized for highly anisotropic tensor and $S \neq 1/2$. In the presence of static magnetic field $\boldsymbol{B}_0 \parallel z$ and resonant transverse MW field $\boldsymbol{B}_1 \cos\omega_0 t \parallel x$ $(B_0 \gg B_1)$, the Hamiltonian of a system of spins coupled by MD interactions is as follows:

$$H = H_0 + H_1 + V = \sum_j \left(H_0^j + H_1^j \right) + \frac{1}{2} \sum_{j \neq k} V^{jk}, \tag{3}$$

where $H_0^j = \hbar\omega_j S_z^j$, $H_1^j = 2\hbar\Omega_R S_x^j \cos\omega_0 t$, and $V^{jk} = \hbar \sum_{\alpha,\beta=x,y,z} A^{jk}_{\alpha\beta} S^j_\alpha S^k_\beta$ is MD interaction between j-th and k-th spins connected by radius-vector $r_{jk}\,(x_{jk}, y_{jk}, z_{jk})$. We suppose that Larmor precession frequencies of spins are distributed around ω_0 in the inhomogeneously broadened resonance line of standard deviation σ. At the moment $t = 0$ when the MW field is turned on, the spin system is described by the initial density matrix of the form

$$\rho(0) \approx \frac{1}{2^N} \prod_j \left(1 - \frac{\hbar\omega_0 S_z^j}{k_B T} \right), \tag{4}$$

where N is the number of spins, T is the temperature of thermostat, k_B is Boltzman constant, and $\hbar\omega_0 \ll k_B T$. A transformation of Eq. (3) into the reference frame RF rotating around z axis of laboratory reference frame LF with the frequency ω_0 yields

$$\begin{gathered} H' \simeq \hbar \textstyle\sum_j \left(\delta\omega_j S_z^j + \Omega_R S_x^j \right) + \\ + \frac{\hbar}{2} \textstyle\sum_{j \neq k} A^{jk}_{zz} \left(S_z^j S_z^k - \frac{1}{2} S_x^j S_x^k - \frac{1}{2} S_y^j S_y^k \right), \end{gathered} \tag{5}$$

where $\delta\omega_j = \omega_j - \omega_0$ is the shift of Larmor frequency of j-th spin from resonance, and we have omitted oscillating time-dependent terms in H'. Let us perform an additional rotation around y axis of j-th ion $(j = \overline{1, N})$ such that new local $\tilde{x}^j$ axis points in the direction of residual external field in RF. The spin projections onto this new set of local axes $\tilde{x}^j, \tilde{y}^j, \tilde{z}^j$ are:

$$\begin{gathered} \tilde{S}_x^j = \left(\Omega_R S_x^j + \delta\omega_j S_z^j \right)/\Omega_j, \qquad \tilde{S}_y^j = S_y^j, \\ \tilde{S}_z^j = \left(\Omega_R S_z^j - \delta\omega_j S_x^j \right)/\Omega_j. \end{gathered} \tag{6}$$

The Hamiltonian (5) written in new spin projections is

$$H' = \hbar \sum_j \Omega_j \tilde{S}^j_x + \frac{\hbar}{2} \sum_{\alpha\beta; j\neq k} \tilde{A}^{jk}_{\alpha\beta} \tilde{S}^j_\alpha \tilde{S}^k_\beta, \qquad (7)$$

where $\Omega_j = \sqrt{\delta\omega_j^2 + \Omega_R^2}$ is the nutation frequency of j-th spin detuned by $\delta\omega_j$ from resonance. In the case of sufficiently small spin concentrations, we leave only the $\tilde{S}^j_x \tilde{S}^k_x$ terms of MD interaction in Eq. (7) that are secular to the interaction with the external magnetic field in *RF*. As we will see, these terms result in random shifts of spin nutation frequencies. We neglect nonsecular terms responsible for mutual spin flip-flops that are significant only when the average local field at the spin site induced by nearby spins is comparable to σ. The response of a spin system on the driving resonant MW field is given by time evolution of its magnetic moment (μ_B is Bohr magneton):

$$\boldsymbol{M}(t) = g_e \mu_B \mathrm{Tr} \left\{ e^{-iH't/\hbar} \rho(0) e^{iH't/\hbar} \sum_j \boldsymbol{S}^j \right\}. \qquad (8)$$

It is easier to calculate the trace in Eq. (8) in the basis of $\tilde{S}^j_x$ eigenfunctions $|\pm 1\rangle = (|\uparrow\rangle \pm |\downarrow\rangle)/\sqrt{2}$ rather than $\tilde{S}^j_z$ eigenfunctions $|\uparrow\rangle, |\downarrow\rangle$. The terms linear in $\delta\omega_j$ disappear after the average over the spectral position ω_j of j-th spin in the symmetric resonance line centered at ω_0. For instance, y-projection $M_y(t)$ equals:

$$M_y(t) = -\frac{g_e \mu_B \hbar \omega_0 \Omega_R}{2^{N+1} k_B T} \sum_j \Omega_j^{-1} \times$$
$$\times \sum_{\{m_l\}'} \sin\left[\left(\Omega_j + \frac{1}{2}\sum_{k(\neq j)} \tilde{A}^{jk}_{xx} m_k\right) t\right], \qquad (9)$$

where $\{m_l\}' = (m_1, \dots, m_{j-1}, m_{j+1} \dots, m_N)$ denotes the configuration of $N-1$ spins with spin projections $m_l = \pm 1$. The obtained expression is intuitively obvious: the j-th spin oscillates around $\tilde{x}^j$ axis in *RF* with frequency $\Omega_j + \frac{1}{2}\sum_{k(\neq j)} \tilde{A}^{jk}_{xx} m_k$. The shift $\tilde{A}^{jk}_{xx} m_k/2$ of its nutation frequency originates from the local field at its site induced by the k-th spin in state $|m_k\rangle$. Performing summation over all possible spin configurations $\{m_l\}'$, we obtain:

$$M_y(t) = \frac{M_0 \Omega_R}{N} \sum_j \frac{\sin \Omega_j t}{\Omega_j} \prod_{k(\neq j)} \cos\left(\tilde{A}^{jk}_{xx} t/2\right), \qquad (10)$$

where $M_0 = -\frac{N g_e \mu_B \hbar \omega_0}{4 k_B T}$ is the initial magnetization of the spin system. The factor $\prod_{k(\neq j)} \cos\left(\tilde{A}^{jk}_{xx} t/2\right)$ in Eq. (10) is responsible for the damping of RO because of MD interactions. We assume that (i) spins occupy random positions $\boldsymbol{r}_k$ within the volume V, (ii) their frequencies ω_k are distributed within the symmetric resonance line of spectral density $g(\omega_k)$ centered at ω_0, (iii) $\boldsymbol{r}_k$ and ω_k do not correlate. The averaging over $\boldsymbol{r}_k$ and ω_k in the limit $N, V \longrightarrow \infty$ yields:

$$\prod_{k(\neq j)} \left\langle \cos\left(\tilde{A}^{jk}_{xx} t/2\right)\right\rangle_{\boldsymbol{r}_k, \omega_k} = \left\{1 - \frac{C}{N}\int d\omega_k g(\omega_k) \times \right.$$
$$\left. \times \int_\infty d^3 r_{jk} \left[1 - \cos\left(\tilde{A}^{jk}_{xx} t/2\right)\right]\right\}^{N-1} =$$
$$= \exp\left\{-C \int d\omega_k g(\omega_k) \int_\infty d^3 r_{jk} [1 - \cos(\tilde{A}^{jk}_{xx} t/2)]\right\}, \qquad (11)$$

where $C = N/V$ is the spin concentration. Substituting

$$\tilde{A}^{jk}_{xx} = \frac{g_e^2 \mu_B^2}{\hbar r_{jk}^5 \Omega_j \Omega_k} \left(r_{jk}^2 - 3 z_{jk}^2\right)\left(\delta\omega_j \delta\omega_k - \frac{1}{2}\Omega_R^2\right)$$

and performing the integration over $\boldsymbol{r}_{jk}$ in Eq. (11), one obtains

$$M_y(t) = M_0 \int d\omega_j g(\omega_j) \frac{\Omega_R}{\Omega_j} \sin \Omega_j t \times$$
$$\times \exp\left\{-\Delta\omega_d t \int d\omega_k g(\omega_k) \frac{|\delta\omega_j \delta\omega_k - \Omega_R^2/2|}{\Omega_j \Omega_k}\right\}, \qquad (12)$$

where $\Delta\omega_d = 4\pi^2 g_e^2 \mu_B^2 C / \left(9\sqrt{3}\hbar\right)$ is known as the static half-width of the resonance line due to MD interactions [21]. In other words, $\Delta\omega_d$ is the average z-component of local magnetic field at a spin produced by neighboring spins. The above statement that non-secular parts of MD interactions are negligible as compared with secular ones corresponds to the condition $\Delta\omega_d \ll \sigma$ which is typically valid when $C < 10^{19}$ ions/cm^3. Given the line shape $g(\omega)$, one can calculate numerically the average magnetization (12) for the given values of C, Ω_R and σ. However, it is possible to obtain analytical expressions for $M_y(t)$ in two practically important approximations:

a) The case of weakly inhomogeneously broadened resonance line (or high MW field): $\sigma \ll \Omega_R$. All spins in the line nutate with the same frequency Ω_R, and

$$M_y(t) = M_0 e^{-\Delta\omega_d t/2} \sin \Omega_R t. \qquad (13)$$

Thus, when the resonance line is fully excited, MD interactions cause exponential decay of RO with the rate $\tau_R^{-1} = \Delta\omega_d/2$ independent of Ω_R.

b) Strongly inhomogeneously broadened resonance line (weak MW field): $\sigma \gg \Omega_R$. The resonance line is partially excited. Roughly, only the spins with Larmor frequencies falling into the range $[\omega_0 - \Omega_R, \omega_0 + \Omega_R]$ are involved in RO. At sufficiently small spin concentrations, the condition $\Omega_R \gg \Delta\omega_d$ is also valid. When $\sigma t \gg 1$, i.e. almost immediately after the transient regime is turned on,

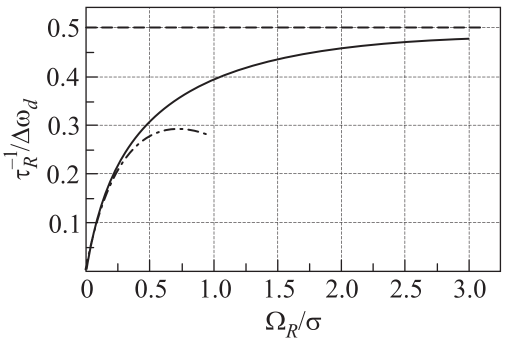
$$M_y(t) = \pi M_0 g(\omega_0)\,\Omega_R e^{-\beta_d \Omega_R t} J_0(\Omega_R t). \tag{14}$$

It is remarkable that the parameter β_d in Eq. (14) has the same form for both Gaussian $g_G(\omega) = \left(2\pi\sigma^2\right)^{-1/2} \exp\left[-\delta\omega^2/2\sigma^2\right]$ and Lorentzian $g_L(\omega) = \sigma/\left[\pi\left(\delta\omega^2 + \sigma^2\right)\right]$ distributions:

$$\beta_d = \Delta\omega_d g(\omega_0) \ln\frac{2\sigma}{\Omega_R}. \tag{15}$$

In general, there may be several spin components with different resonance frequencies (e.g. in case of hyperfine structure of ESR line). Then, we must replace $\Delta\omega_d$ with $\kappa\Delta\omega_d$ in all above expressions, where $\kappa \le 1$ is the fraction of spins belonging to the given resonance line.

When $\sigma \sim \Omega_R$, the problem can be approached numerically. Results of numeric calculations of the decay rate obtained from Eq. (12) (assuming one spin component and Gaussian line shape) for arbitrary values of Ω_R/σ, together with the asymptotic solutions for $\sigma \ll \Omega_R$ and $\sigma \gg \Omega_R$, are presented in Figure. For sufficiently small experimental range of Ω_R/σ, we can



The dependence of decay rate τ_R^{-1} of transverse magnetization on Rabi frequency Ω_R calculated from Eq. (12) assuming one spin component and Gaussian line shape (solid line). The asymptotes $\tau_R^{-1} = \Delta\omega_d/2$ for $\sigma \ll \Omega_R$ and $\tau_R^{-1} = \Delta\omega_d g_G(\omega_0)\,\Omega_R \ln\frac{2\sigma}{\Omega_R}$ for $\sigma \gg \Omega_R$ are represented by dashed and dash-dotted lines, respectively

approximate the decay rate in Figure by a line segment (cf. Eq. (2)):

$$\tau_R^{-1} = \alpha_d + \beta_d \Omega_R. \tag{16}$$

Here the constant term α_d is approximately zero for $\Omega_R/\sigma \ll 1$, approaches $\kappa\Delta\omega_d/2$ for $\Omega_R/\sigma \gg 1$, and

$$\beta_d = \frac{\kappa\Delta\omega_d \mathrm{tg}\psi}{\sigma} \equiv \gamma_d C, \qquad \gamma_d = \frac{4\pi^2 g_e^2 \mu_B^2 \kappa \mathrm{tg}\psi}{9\sqrt{3}\hbar\sigma}, \tag{17}$$

where ψ is the averaged slope angle of the function $F(x) = \tau_R^{-1}(x)/\Delta\omega_d$, $\mathrm{tg}\psi = dF/dx$ (see Figure) in the given experimental range of $x = \Omega_R/\sigma$.

RO are detected in experiment either through transverse $M_\perp(t) = M_y(t)$ (e.g. two-photon resonance technique [13, 14]) or longitudinal M_z (e.g. transient pulse followed by spin echo sequence [15]) magnetization. Performing calculations analogous to Eqs. (9)–(14) assuming again that $\Delta\omega_d \ll \sigma, \Omega_R$, one obtains time-dependent part of longitudinal magnetization:

$$M_z(t) = \begin{cases} M_0 e^{-\Delta\omega_d t/2} \cos\Omega_R t, & \sigma \ll \Omega_R, \\ \pi M_0 g(\omega_0)\,\Omega_R e^{-\beta_d \Omega_R t} j_0(\Omega_R t), & \sigma \gg \Omega_R, \end{cases} \tag{18}$$

where $j_0(z) = \int_z^\infty J_0(z)\,dz$.

Particularly interesting is the case of strong inhomogeneity $\sigma \gg \Omega_R$ common in ESR. There, after a number of oscillations, i.e. $\Omega_R t \gg 1$, one can use asymptotic representation $j_0(z \gg 1) \simeq J_0(z + \pi/2) \simeq \sqrt{2/(\pi z)}\cos(z + \pi/4)$. In this case, there appear two contributions into RO decay:

(i) Polynomial damping $\sim (\Omega_R t)^{-1/2}$. Different static shifts $\delta\omega_j$ lead to different nutation frequencies Ω_j that result in mutual dephasing of spins during RO. This contribution is well-known in the field of magnetic resonance (see, e.g., [2]) and does not lead to decoherence of spin states. It is absent in the case of weak inhomogeneity $\sigma \ll \Omega_R$.

(ii) Exponential damping $\sim e^{-\beta_d \Omega_R t}$. This contribution reflects decoherence inside a bath of equivalent spins coherently driven by resonant MW field and coupled by MD interactions. Since β_d depends on Ω_R through slowly-varying logarithmic function (see Eq. (15)), the damping rate (16) is approximately linear in Rabi frequency in the specific range of Ω_R. When $\sigma \ll \Omega_R$, the damping rate is independent of Ω_R, cf. Eq. (13).

It is noteworthy to compare our results with the experimental data on anomalous decay of RO in ESR [13, 14, 17]. In view of all above-mentioned, we address Ω_R-dependent term in Eq. (2) to relaxation induced by MD interactions between the spins of the same resonant line coherently driven by MW field (the second term in Eq. (16)). The constant term in Eq. (2) (usually indistinguishable) corresponds to the first term in Eq. (16) and other spin relaxation processes that do not depend on Ω_R (e.g. spin-lattice interaction).

Spin centers	C, 10^{16} cm^{-3}	β, 10^{-2}	β_d, 10^{-2}	$\beta_0+\beta_d$, 10^{-2}
E_1'	7.5 ± 2	4.8 ± 0.5	0.94 ± 0.25	5.7
	16 ± 5	6.1 ± 0.5	2.00 ± 0.63	6.4
	24 ± 8	10.6 ± 0.5	3.00 ± 1.00	9.0
$[\mathrm{AlO_4}]^0$	4.0 ± 0.4	2.4 ± 0.1	0.17 ± 0.02	2.30
	1.0 ± 0.1	2.1 ± 0.1	0.043 ± 0.004	2.15

Measured (β, [13, 14]) and calculated ($\beta_d = \gamma_d C$, this work) RO decay parameters for E_1' centers in glassy silica and $[\mathrm{AlO_4}]^0$ centers in quartz. ESR lines were approximated by Gaussian distribution with experimental standard deviations $\sigma(E_1') = 2\pi \cdot 1\,\mathrm{MHz}$, $\sigma([\mathrm{AlO_4}]^0) = 2\pi \cdot 0.25\,\mathrm{MHz}$ [13, 14]. The γ_d values for each system were calculated according to Eq. (17), resulting in $\gamma_d(E_1') = 1.25 \cdot 10^{-19}\mathrm{cm}^3$ and $\gamma_d([\mathrm{AlO_4}]^0) = 4.3 \cdot 10^{-20}\mathrm{cm}^3$. The last column represents the best fit of β within the concentration error bounds by the function $\beta = \beta_0 + \beta_d$, with $\beta_0(E_1') = 5 \cdot 10^{-2}$ and $\beta_0([\mathrm{AlO_4}]^0) = 2.11 \cdot 10^{-2}$.

In order to reveal the importance of the above decay mechanism in transient response of real systems, we have calculated RO decay rates according to Eqs. (16), (17) for E_1' and $[\mathrm{AlO_4}]^0$ centers and compared them to the ones observed in [13, 14]. Transient nutations of E_1' centers in glassy silica and $[\mathrm{AlO_4}]^0$ centers in quartz had been detected by means of two-photon ESR at resonance frequency $\omega_0 = 2\pi \cdot 5.9\,\mathrm{GHz}$ [13, 14]. The measured RO decay parameters β are found to be well approximated within experimental error bounds by the sum $\beta = \beta_0 + \beta_d$ (see Table), where the constant term β_0 probably originates from the MW field inhomogeneities inside the sample volume [10]. Our model predicts that for spin concentrations $C > 5 \cdot 10^{17}\mathrm{cm}^{-3}$ in both systems β_d will prevail over β_0. The calculated values of β_d agree very well with the concentration-dependent parts of β (cf. columns 4 and 6 in Table), which experimentally validates the RO decay mechanism considered in the present paper.

To summarize, we performed first-principles calculations of the relaxation processes occurring in dipolar-coupled A spin bath during transient regime. We have shown that the decoherence in A spin bath, under specific conditions, is enhanced by the external resonant microwave field, in contrast with B spin bath. The decay rate of Rabi oscillations depends linearly on the concentration of magnetic impurity and, in the strong inhomogeneity case, almost linearly on Rabi frequency. The obtained results are of importance for the implementation of many-qubit systems in quantum information processing.

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1. I. I. Rabi, Phys. Rev. **51**, 652 (1937).
2. H. C. Torrey, Phys. Rev. **76**, 1059 (1949).
3. P. W. Atkins, A. J. Dobbs, and K. A. McLauchlan, Chem. Phys. Lett. **25**, 105 (1974).
4. G. B. Hocker and C. L. Tang, Phys. Rev. Lett. **21**, 591 (1968).
5. R. M. Rakhmatullin, I. N. Kurkin et al., Phys. Rev. B **79**, 172408 (2009).
6. S. Bertaina, S. Gambarelli, T. Mitra et al., Nature **453**, 203 (2008).
7. D. P. DiVincenzo, Science **270**, 255 (1995).
8. J. I. Cirac and P. Zoller, Phys. Rev. Lett. **74**, 4091 (1995).
9. J. J. L. Morton, A. M. Tyryshkin et al., Phys. Rev. A **71**, 012332 (2005).
10. E. I. Baibekov, I. N. Kurkin, M. R. Gafurov et al., J. Magn. Res. **209**, 61 (2011).
11. A. Abragam, *The Principles of Nuclear Magnetism*, Clarendon Press, Oxford, 1961.
12. A. Abragam and B. Bleaney, *Electron Paramagnetic Resonance of Transition Ions*, Oxford Univ. Press, London, 1970.
13. R. Boscaino, F. M. Gelardi, and J. P. Korb, Phys. Rev. B **48**, 7077 (1993).
14. S. Agnello, R. Boscaino, M. Cannas et al., Phys. Rev. A **59**, 4087 (1999).
15. S. Bertaina, S. Gambarelli, A. Tkachuk et al., Nature Nanotech. **2**, 39 (2007).
16. S. Nellutla, K.-Y. Choi, M. Pati et al., Phys. Rev. Lett. **99**, 137601 (2007).
17. J. H. Shim, S. Gambarelli, S. Bertaina et al., arXiv:1006.4960v2.
18. R. N. Shakhmuratov, F. M. Gelardi, and M. Cannas, Phys. Rev. Lett. **79**, 2963 (1997).
19. N. Ya. Asadullina, T. Ya. Asadullin, and Ya. Ya. Asadullin, J. Phys.: Cond. Matter **13**, 3475 (2001).
20. B. Herzog and E. L. Hahn, Phys. Rev. **103**, 148 (1956).
21. W. B. Mims, Phys. Rev. **168**, 370 (1968).
22. V. V. Dobrovitski, A. E. Feiguin, R. Hanson, and D. D. Awschalom, Phys. Rev. Lett. **102**, 237601 (2009).
23. P. C. E. Stamp and I. S. Tupitsyn, Phys. Rev. B **69**, 014401 (2004).