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Magnetization Dynamics of a Material with Spin Triplet States Affected by a Weakly Varying Field and Spin-Lattice Interaction in a Zero Constant Field

Dr.Srinivas Bachu[1], Professor[1], Department of ECE, Siddhartha Institute of Technology & Sciences, Telangana, India

Vijay Koraveni[2], Assistant Professor[2], Department of CSE, Siddhartha Institute of Technology & Sciences, Telangana, India.

ABSTRACT

The goal of this researchchanged into to have a look ateachnormal and abnormal dynamics of spin-triplet states (STSs) withinside the case of one-photon and one-magnon interactions with the various magnetic subject and the lattice, respectively. The anisotropic normal dynamics of STSs of molecular unmarried crystals in 0steady and vulnerablevarious magnetic fields (weak spotapproach the absence of saturation on theconsistentnation and of the nutation on the pulse EPR) directed alongside the molecular axes, changed into analytically investigated. The equations have been derived for the unfastenedmovement of the pattern magnetization, describing its linear oscillations alongside that molecular axis, alongside which its nonzero preliminarypricechanged into created. The tensor of the consistent-nation dynamical susceptibility to the varioussubjectchanged into found. The end result of the motion of a quick MW pulse on STS changed into analytically described, containing a periodic dependence at the pulse period and its detuning. The anisotropic abnormal dynamics of electron spin-lattice relaxation (SLR) at its one-phonon mechanism changed into investigated without the excessive temperature approximation over the phonon temperature; the SLR costs of the separate transitions of STS have been calculated; the corresponding SLR possibilitieshave been written withinside the form, which supposes the fractal dimensionality d of a lattice; the consequences with d=4/three agreed nicely with the experimental statistics in STS of the buried tryptophan of ribonuclease

Keywords:

EPR; spin-triplet states; spin-lattice relaxation; fractal dimensionality.

INTRODUCTION

A spin triplet state (STS) is a quantum state of a system with a spin of quantum number S=1. The photoexcited (PE) linear polyarene molecules in mixed organic crystals, triplet excitons, Cu2+ dimers in metal-oxide complexes, and nitrogen nuclei possess such states. PE amino acids in different proteins and other bio-objects possess STS,
too. All these materials play important role in science and technique [1]. Organic crystals with STS are used in optoelectronics and in electromagnetic devices, such as flexible OLED (organic light-emitting diodes), solar cells, and masers. Low cost
and simple manufacturing are their advantages. It is worth noting that STS of PE pentacene in mixed molecular crystals can be successfully applied for the investigation at room temperature of such new conceptions, as quantum oscillations of nuclear spins and spin entanglement, the latter being important for quantum algorithms. It is self-evident that the success of abovementioned applications is based on the deep insight into the physics of STS. EPR is a powerful tool for the investigation of the dynamics of STS. At that, it is a well-known method of the non-destructive testing of materials. A great number of EPR experiments on STS with the zero-field splitting (ZFS) of their levels were made in zero constant field [1-5]. The sensitivity of ZFspectroscopy to small shifts in local magnetic fields enables the studies of the effects of the guesthost interactions in diluted organic paramagnets over a wide temperature range [3,4].

The modest size of the spectrometer without a large magnet, creating constant field, is a significant preference of ZF EPR [1]. As in the usual EPR, so in ZF EPR the observation of the STS response to their excitement by the microwave (MW) field takes place. This response can be free (after the MW cut-out) and steady state; besides, the investigation of the spin-lattice relaxation (SLR) is possible with the help of this response. As soon as this response is the reflection of the motion of the full magnetization of the sample, the importance of the obtaining of the equations describing the motion of the components of this magnetization is obvious. The obtaining of such equations at the weak MW field directed along the molecular axes X, Y, Z is one of the tasks of the given paper. The "weakness" of the varying field means that here we use the linearized equations for the sample magnetization, i.e., we exclude from the consideration the saturation of the transitions of the ZFS at the steady state and the nutation at the pulse EPR. In addition, the investigation of the spin-lattice relaxation anisotropy on the separate transitions of ZFS in the case of the one-phonon mechanism of relaxation, dominating in experiments of [5], is the purpose of this work.

At that, our aim was to check the validity of the supposition of the authors of [5] about the fractal dimensionality of ribonuclease: i.e., to calculate the probabilities of the relaxational transitions between

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the levels of ZFS of the buried tryptophan residue of ribonuclease (RNase) T1 and to compare the results with the experimental data of [5]. At that, we shall consider only the case of a linear lattice, and exclude from consideration the case of a nonlinear lattice with the associated possibility of the existence of discrete breathers [6], though the latter case was assumed to be present in myoglobin "lattice", similar to the RNase "lattice", by the authors of Ref. [7]. In addition, we shall not consider the nanomagnets with the "fractal" structure (as an example of such structures, see Fig.1).

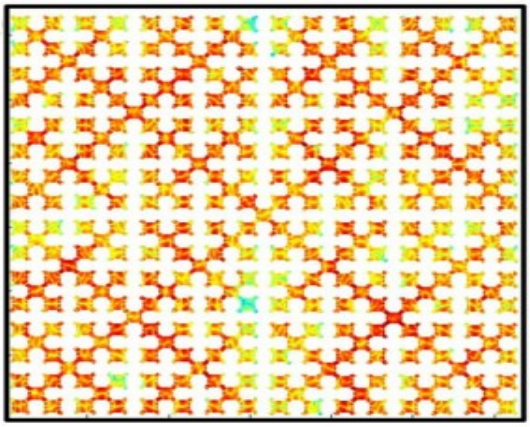

Fig. 1. Example of the fractal structure of Permalloy Ni80Fe20 nanomagnet (copy of Fig. 18 from [8])

RESULTS AND DISCUSSION

With the help of the single transition operators (STOs) [9-12] the following exact equations of the free motion of the magnetization M, M, M X Y Z M () of a sample with STS in zero constant field can be obtained:

$$\ddot{M}_X+(Y-Z)^2\hbar^{-2}M_X=0$$
$$\ddot{M}_Y+(Z-X)^2\hbar^{-2}M_Y=0 \qquad (1)$$
$$\ddot{M}_Z+(X-Y)^2\hbar^{-2}M_Z=0$$

where

$$X=D/3-E;\quad Y=D/3+E;\quad Z=-(2/3)D$$

are the energies of the STS levels; D E, are the parameters of ZFS, the latter hereafter in this paper is supposed to be well resolved. It should be noted that, as it was expected, these equations do not follow from the corresponding equations for the motion of the magnetization components in the sufficiently strong magnetic field, obtained in [11], at the vanishing value of this field. The following anisotropic character of STS free motion is seen from equations (1): each component of the sample magnetization M, M, M X Y Z under conditions of creating its non-zero initial value, accomplishes the linear oscillation along the corresponding axis. This conclusion coincides with the text of § 5 of the Chapter 3 of Abraham, Bleany monograph [13]. These oscillations have frequencies $\omega_0^{i-j}=\pm\left|\omega_0^{i-j}\right|$, where $i,j=X,Y,Z$ are the energy levels of STS; $\omega_0^{Y-Z}\equiv(Y-Z)/\hbar=(D+E)/\hbar;\omega_0^{Z-X}\equiv(Z-X)/\hbar=(-D+E)/\hbar;\omega_0^{X-Y}\equiv(X-Y)/\hbar=-2E/\hbar.$

The evolution of magnetization of a sample with STS in a zero-constant field under the action of a weak MW field, directed along the K -th axis, is described by the unitary transformed (see Ref. [10]) Hamiltonian $\mathcal{H}_{sh}^{*}=2g_{\mathbf{K}}^{i-j}\mu_B B_{1\mathbf{K}}^{i-j}S_{\mathbf{Y}}^{i-j}$ cos Wt and leads to the following approximate equations:

$$\ddot{M}_{\mathbf{K}}+2\left(T_{2\mathbf{K}}^{*}\right)^{-1}\dot{M}_{\mathbf{K}}+\left(\omega_0^{i-j}\right)^2M_{\mathbf{K}}=\pm g_{\mathbf{K}}\mu_B\hbar^{-1}\left|\omega_0^{i-j}\right|\left(-n_{\alpha}g_{\mathbf{K}}\mu_B\right)P_{\alpha}^{i-j}\cdot 4B_{1\mathbf{K}}^{i-j}\cos\omega t. \qquad (2)$$

here

$$\mathbf{K}\,i,j=\mathbf{X},Y,Z=\mathbf{Y},Z,X=\mathbf{Z},X,Y\;;\;2B_{1\mathbf{K}}^{i-j}$$ cos

1 I j B ωt – K is the value of the linear polarized MW field; I j g – K are the diagonal components of the g -factor tensor of STS; i j S – Y are STOs related to the transition between the i and j levels; ex n is the concentration of the photo-excited molecules, μ B is the Bohr magneton. Under conditions of the weak MW field, which cannot cause the saturation of the steady state EPR and the nutation at the pulse EPR, the values i j i j P P P ex ex ex –≡– are the population differences of the photo-excited STS levels at the absence of MW field. It is seen from these equations that the forced linear oscillations of the K -th component MK of the full sample magnetization are induced by the MW field, polarized along the K -th axis.

The decay rates $\left(T_{2\mathbf{X},\mathbf{Y},\mathbf{Z}}^{*}\right)^{-1}$ of the magnetization components $M_{\mathbf{X}}$, $M_{\mathbf{Y}}$, $M_{\mathbf{Z}}$ to their zero equilibrium values are introduced in (2) by us phenomenologically. At the given stage, only one paper [14] is known to us, for which the solutions of these equations are directly applicable at the MW frequency sweep. In the sample of this paper (PE naphthalene in diphenyl), the anisotropic inhomogeneous broadening of the steady state EPR lines is conditioned by the unresolved hyperfine interaction (HFI) of STS with the protons of their own molecules. Following [15], we describe the

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decay, caused by the spin distribution over frequencies due to this HFI and other less important broadening causes, by the values $\left(T^{*}_{2\mathbf{X},\mathbf{Y},\mathbf{Z}}\right)^{-1}$ The solving of the Eqs. (2) enables us to write thecomplex tensor of the steady state dynamic susceptibility to the MW field with the frequency ω , directed along the K -th axis:

$$\chi_{\mathbf{KK}'}=\begin{pmatrix}\chi_{XX} & 0 & 0\\ 0 & \chi_{YY} & 0\\ 0 & 0 & \chi_{ZZ}\end{pmatrix}, \qquad (3)$$

where

$$\chi_{\mathbf{KK}}\equiv\chi'_{\mathbf{KK}}-i\,\chi''_{\mathbf{KK}}=\pm\hbar^{-1}g_{\mathbf{K}}^{i-j}\mu_B\mu_0\left(-n_\alpha g_{\mathbf{K}}^{i-j}\mu_B\right)P^{i-j}\frac{\left|\omega_0^{*i-j}\right|-\omega-i\left(T_{2\mathbf{K}}^{*i-j}\right)^{-1}}{\left(\left|\omega_0^{*i-j}\right|-\omega\right)^2+\left(T_{2\mathbf{K}}^{*i-j}\right)^{-2}}, \qquad (4)$$

the signs ± in (4) correspond to the signs of the values $\omega_0^{*i-j}=\pm\left|\omega_0^{*i-j}\right|$; $\left|\omega_0^{*i-j}\right|$ are the center frequencies of the ZFS transitions, shifted by HFI in the situation of [14], μ0 is the magnetic constant. However, the pulse ZF EPR is of the main interest and actuality [1-4]. Here, we would like to consider the result of the action on STS of a sufficiently weak and short MW pulse (which is not able to cause the nutation of the single transition spin vector) of the MW field. The following values of the magnetization MK (tp) , created by the exciting pulse of the MW field of p t duration along the K -th axis, can readily be obtained from the Eq. (2) with the help of the corresponding formula from [16]:

$$M_{\mathbf{K}}\left(t_p\right)=\pm\frac{\left(-n_\alpha g_{\mathbf{K}}^{i-j}\mu_B\right)P_\alpha^{i-j}\left(g_{\mathbf{K}}^{i-j}\mu_B\hbar^{-1}\right)\cdot 4B_{1\mathbf{K}}^{i-j}}{\sqrt{\left(\left|\omega_0^{*i-j}\right|-\omega\right)^2+\left(T_{2\mathbf{K}}^{*i-j}\right)^{-2}}}\sin\left[\left(\left|\omega_0^{*i-j}\right|-\omega\right)t_p/2\right]\sin\left(\left|\omega_0^{*i-j}\right|t_p\right) \qquad (5)$$

If $\left(T_{2\mathbf{K}}^{*i-j}\right)^{-1}=0$, the periodic dependencies of $M_{\mathbf{K}}\left(t_p\right)$ envelope value as on the detuning, so on the exciting pulse duration are seen from (5). At that, these dependencies have the different form for the different i-j transitions. We now turn to the problem of spin-lattice relaxation, where the unitary transformed (see Ref. [10]) perturbation has the form $\mathcal{H}^{*}_{sph}=U_0\mathcal{H}_{sph}U_0^{-1}=2\sum_{\alpha\beta}e_{\alpha\beta}\left\{\mathcal{G}^{\mathbf{X}}_{\alpha\beta}S_{\mathbf{Y}}^{Y-Z}+\mathcal{G}^{\mathbf{Y}}_{\alpha\beta}S_{\mathbf{Y}}^{Z-X}+\mathcal{G}^{\mathbf{Z}}_{\alpha\beta}S_{\mathbf{Y}}^{X-Y}\right\}$, $\alpha,\beta=\mathbf{X},\mathbf{Y},\mathbf{Z}$; $e_{\alpha\beta}$ s the crystal deformation tensor component; αβ K G are the constants of the spinphonon bond. Just as the STS interaction with the varying field directed along the K -th axis of the form $\mathcal{H}^{*}_{sh}=2g_{\mathbf{K}}^{i-j}\mu_B B_{1\mathbf{K}}^{i-j}S_{\mathbf{Y}}^{i-j}\cos\omega t$ causes transitions between the i-j levels of STS, described by regular dynamics, so the STS interaction with the lattice of the form $2e_{\alpha\beta}\mathcal{G}^{\mathbf{K}}_{\alpha\beta}S_{\mathbf{Y}}^{i-j}$, causes the same transitions, however described by the irregular dynamics. For the calculation of the probabilities of the one-phonon SLR transitions between the triplet levels it is convenient to start with the finding of the SLR rate T_{sph}^{-1} of the entire spin system of the STSs, which is characterized by a single spin temperature. The spins with a non-equidistant spectrum can have a single spin temperature in two cases: when they are in equilibrium with the lattice, and when they have infinite spin temperature. In the first case, the measurement of the SLR rate T_{sph}^{-1} between i-j levels of a spin-triplet system is possible by the Gorter method. In this case, the maximum of the absorption signal of the low-frequency ω field directed along the K -th axisThe SLR rates of the i-j transition without the high temperature approximation over phonon temperature, according to the formula (5.6) [22], rewritten for STS, have the form:

$$\left(T_{sph}^{i-j}\right)^{-1}=W_{ij}+W_{ji}+\frac{1}{2}\left(W_{j\mathbf{K}}+W_{\mathbf{K}j}\right)+\frac{1}{2}\left(W_{\mathbf{K}i}+W_{i\mathbf{K}}\right), \text{ or}$$

$$\left(T_{sph}^{i-j}\right)^{-1}=\frac{2\pi^2nd}{k_BT_L\hbar^{d+1}\left(6\pi^2n\right)^{d/3}}\times\sum_{\alpha,\beta}L_{\alpha\beta}\left\{2\left(\mathcal{G}^{\mathbf{K}}_{\alpha\beta}\right)^2\left|E_i-E_j\right|^d cth\left(\left|E_i-E_j\right|/2k_BT_L\right)+\right.$$

$$\left.+\left(\mathcal{G}^{i}_{\alpha\beta}\right)^2\left|E_j-E_K\right|^d cth\left(\left|E_j-E_K\right|/2k_BT_L\right)+\left(\mathcal{G}^{j}_{\alpha\beta}\right)^2\left|E_K-E_i\right|^d cth\left(\left|E_K-E_i\right|/2k_BT_L\right)\right\}$$

Taking into account the experimental data for the buried tryptophan residue in RNase T1 in 40% glycerol-phosphate buffer mixture from [5] with the ZFS parameters D GHz E GHz ≈≈ 2.9 , 1.3 [23], and also the value of the fractal

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dimensionality d = 4 / 3 for RNase [24], the temperature dependencies of the probabilities of the separate relaxation transitions are plotted in Fig. 3, which agree well with the experimental points. It can be seen from Fig. 3 that the correlation / 1.7 W W YZ YX ≈ , which is observed in the experiment, is fulfilled with a good accuracy over the temperature range investigated.

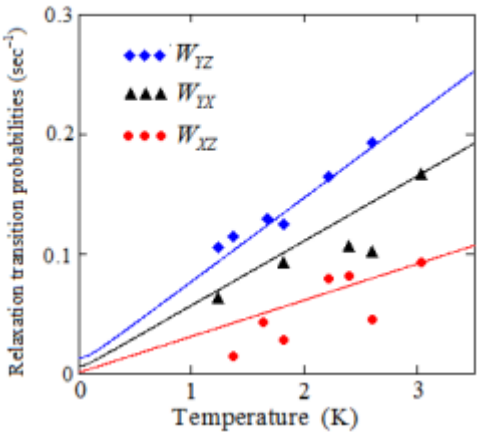

Fig. 3. The temperature dependence of the relaxation transition probabilities for the buried tryptophan residue in RNase T1. The points, triangles and squares are the experimental points from Ref. [5]. The solid lines are plotted according to the analytics of the given paper at the fractal dimensionality d=4/3.

CONCLUSION

Summarizing, the following results on the anisotropic regular spin dynamics of STS of a single crystal in a zero constant magnetic field and a weak varying field, directed along the molecular axes X,Y,Z are obtained: The equations of the free motion of the magnetization of the sample, possessing STS, are derived, describing its linear oscillation along that axis of ZFS, along which its nonzero initial value was created; The tensor of the steady state dynamic susceptibility to a varying field is found; At the absence of nutation, the result of the action of the short pulse of a varying field is found to have a periodic dependence on the pulse duration and on the detuning of the pulse frequency with respect to the transition frequency; The abovementioned results can be applied also to I=1 NMR, what is important for nitrogencontaining explosives and narcotics monitoring. The anisotropic irregular dynamics of STS, namely the SLR of the electron STS at its one-phonon mechanism is investigated without HTA over the phonon temperature: The expressions for the SLR probabilities of separate ZFS transitions are found to be proportional to the d power of the splitting of the corresponding transitions at temperatures close to 0o K. The successful comparison is carried out with the corresponding results of [5] for the buried residue of tryptophan of ribonuclease T1 at low temperatures at d=4/3. At that, the supposition of the authors of [5] about the fractal dimensionality d of RNase T1 is verified

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