

Quasiclassical Model of Spin Diffusion and Relaxation in a Nonuniform Magnetic Field

Gennady P. Berman, Boris Chernobrod, Vyacheslav N. Gorshkov, T-13; and Vladimir I. Tsifrinovich, Polytechnic University

Operation of any quantum spin device crucially depends on the relaxation rate in the spin system. Spin diffusion is recognized as one of the most important factors in a spin relaxation process. The idea of spin diffusion originated from Bloembergen who explained nuclear spin-lattice relaxation in insulating crystals [1]. He demonstrated that the transport of magnetization from fast relaxing spins (FRS) to slow relaxing spins (SRS) can be described by as a diffusion process. Due to the spin diffusion, a small amount of FRS (e.g., located near the impurities) can greatly accelerate the spin-lattice relaxation in the whole spin system. A number of theoretical approaches have been used to describe the spin diffusion. The general theory of the spin diffusion and relaxation in electron spin resonance has been developed in [2].

Recently Budakian, Mamin, and Rugar [3] demonstrated effective manipulation with the electron spin relaxation of E' — centers in silica using the high gradient of the magnetic field produced by a ferromagnetic particle in the magnetic resonance force microscopy.

Inspired by this experiment we have considered a quasiclassical computational model [4] that allows us to simulate the process of spin diffusion and relaxation in the presence of a highly nonuniform magnetic field. The energy of the SRS flows to the FRS due to the dipole-dipole interaction between the spins.

Our computations show that in case of the uniform external magnetic B_z field the overall relaxation time τ_r can be described by the relation

$$\tau_r \approx \frac{\tau_0}{1 + \beta / (\alpha N)},$$

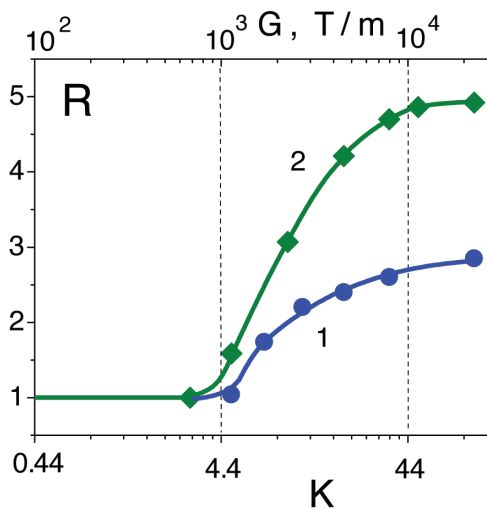
where α is the parameter of relaxation of the SRS, $\beta \gg \alpha$ is that for the FRS, $N \approx n_S/n_F \gg 1$, n_F and n_S are the concentrations of FRS and SRS, τ_0 is the time of relaxation in the absence of the FRS.

The suppression of the relaxation process depends on parameter,

$$K = a \frac{\partial B_z}{\partial z} \left/ \frac{\mu_0 \mu_B}{4\pi a^3} \right.,$$

which is the ratio of the Larmor frequency difference to the dipole-dipole constant (a is the average distance between the spins). The significant increase of the relaxation time τ_r appears in the region $4.4 \leq K \leq 44$, which corresponds to the values $10^3 T/m \leq \partial B_z / \partial z \leq 10^4 T/m$ in a good agreement with experiments [3]. (See Fig. 1.) For $K > 44$, the ratio $R(K) = \tau_r(K)/\tau_r(K=0)$ is approaching the value $1 + \beta / (\alpha N)$. It means that the overall relaxation time $\tau_r(K)$ is approaching the expected value τ_0 . We have found that in the absence of the magnetic field gradient ($K = 0$) the

Fig. 1. Dependence $R(K)$ on K . Curves 1–2: $\beta/(\alpha N) = 4, 2$. $G = \partial B_z / \partial z$.



relaxation process spreads randomly in all directions from FRS to SRS. In the presence of the magnetic field gradient the spin diffusion process becomes anisotropic (See Fig. 2). One can see that the relaxation process first develops in the slice containing FRS ($i = 0$), then it spreads to the slices $i < 0$ below the central slice, then it spreads to the upper slices $i > 0$. The reason of the phenomenon has been thoroughly investigated by us [4].

The processes of spin diffusion and relaxation are studied theoretically and numerically for quantum computation applications in our paper [5]. Two possible realizations of a spin quantum computer (SQC) are analyzed: i) a boundary spin chain in a 2-D spin array, and ii) an isolated spin chain. In both cases, spin diffusion and relaxation are caused by a FRS located outside the SQC. We have shown that in both cases the relaxation can be suppressed by an external nonuniform magnetic field. In the second case, our computer simulations have revealed various types of relaxation processes including the excitation of a random distribution of magnetic moments and the formation of stationary and moving domain walls. The region of optimal parameters for suppression of rapid spin relaxation is discussed.

For more information contact Gennady Berman at gpb@lanl.gov.

- [1] N. Bloembergen, *Physica (Utrecht)* **15**, 386 (1949).
- [2] B.E. Vugmeister, *Phys. Stat. Sol. (b)* **90**, 711 (1978).
- [3] R. Budakian, et al., *Phys. Rev. Lett.* **92**, 037205 (2004).
- [4] G.P. Berman, et al., *Phys. Rev. B* **71**, 184409 (2005).
- [5] G.P. Berman, et al., *Cond-mat*: 0503107 (2005).

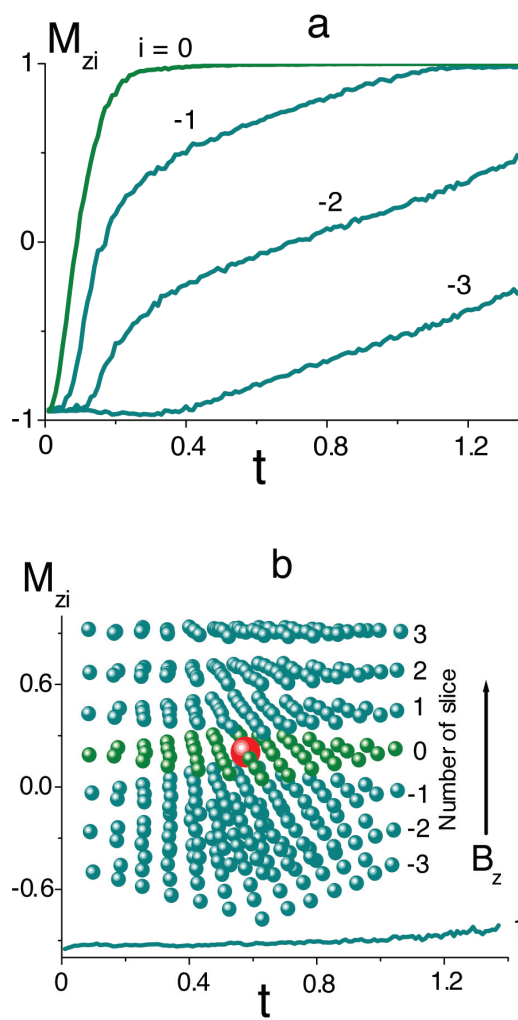


Fig. 2. Relaxation of the slice magnetic moments $M_{zi}(\tau)$ (τ is the dimensionless time) in the presence of the magnetic field gradient: a- for the central slice, which contain FRS ($i = 0$, the red sphere), and for the slices below the central slice; b- for the slice 1 above the central slice. $\beta/(aN) = 4$, $K = 10$.