On the control of the spread of quantum information in multiple quantum NMR spectroscopy of solids

V.E. Zobov[1] and A.A. Lundin[2]

1. Kirensky Institute of Physics, Federal Research Center KSC SB RAS, Krasnoyarsk, 660036 Russia
e-mail: zobov.ve@gmail.com.
2. Semenov Institute of Chemical Physics, Russian Academy of Sciences, Moscow, 117977 Russia
e-mail: ya-andylun2012@yandex.ru

The system of nuclear magnetic moments (spins) of a solid observed by NMR methods is a good example of a closed system. As is known, in a closed system, quantum information is stored with time. Wherein, in the process of time evolution, single-spin correlations turn into multiple-spin correlations due to dipole-dipole interactions. Multiple quantum (MQ) NMR spectroscopy of solids [1] allows us to observe this process and even control it by changing the duration of the intervals of forward and reverse evolutions in time. The form of the MQ spectrum describing the dependence of the intensities of the components on their coherence orders M is well described by the Gaussian distribution, the second moment $<M^2>$ of which determines the average size $\bar{K}$ of the cluster of correlated spins $<M^2>=\bar{K}/2$. Usually, the value $\bar{K}$ from the experimental MQ spectrum is determined through the value of the coherence order M_e, at which the MQ spectrum decreases by "e" times. For the Gaussian function $\bar{K}=2M_e^2$. Crystalline solids such as adamantane and fluorite show rapid growth $\bar{K}$ over time, which is well described by an exponential function $\bar{K}(t)=\exp(at)$. At long times, growth slows down due to decoherence processes, in particular, due to the imperfection of the applied pulse sequence and the created effective Hamiltonian. The authors of [2] proposed introducing a controlled perturbation into the effective Hamiltonian. By changing the magnitude of the perturbation, experimenters were able to control the spread of quantum information and the average size $\bar{K}$. The estimation of the dependence of the stationary value of the size $\bar{K}$ on the magnitude of the perturbation was carried out in [3]. The authors proposed a model with diffusion growth of clusters, in which they took into account their size K distribution and the dependence on K of the rate of cluster degradation caused by perturbation. In [4] and in earlier works, we showed that, in addition to this contribution to degradation, it is important to take into account the contribution to cluster degradation, the rate of which is determined by the order of coherence M. Two such qualitatively different contributions to degradation were observed in adamantane in [5]. To assess the influence of the perturbation on the growth of clusters of correlated spins and on the observed MQ spectra, we implemented an expansion in terms of orthogonal operators, which made it possible to take into account the cluster size K distribution. A simple model with known amplitudes in the absence of perturbation we used for the calculations. The selected model led to exponential growth of $\bar{K}$ with time. Analytical estimates of the effects of perturbation [4] in the proposed report are supplemented by numerical calculations of the MQ spectra and the characteristics: $\bar{K}$, M_e, $<M^2>$. The contribution to the degradation, which depends on the order of coherence, changes the shape of the MQ spectrum. As a result, the ratios of $\bar{K}$ with the values of M_e and $<M^2>$ will change in comparison with those for the Gaussian function. In particular, with an increase in the preparation time, a narrowing of the MQ spectrum can occur while maintaining growth of $\bar{K}$. These changes must be taken into account when extracting the characteristics of the spread of quantum information from experimental MQ spectra.

1. J. Baum, M. Munovitz, A.N. Garroway, and A. Pines. "Multiple-quantum dynamics in solid state NMR". J. Chem. Phys. **83**, pp. 2015-2025, 1985.
2. F.D. Domínguez, M.C. Rodríguez, R. Kaiser, D. Suter, and G.A. Álvarez. "Decoherence scaling transition in the dynamics of quantum information scrambling". Phys. Rev. A, **104**, 012402, 2021.
3. F.D. Domínguez and G.A. Álvarez. "Dynamics of quantum information scrambling under decoherence effects". arXiv:2107.03870, 2021.
4. V.E. Zobov and A.A. Lundin. "Effect of degradation processes caused by a small perturbation on the growth of the average cluster size of correlated spins in multiple quantum NMR spectroscopy of solids". Appl. Magn. Res. **52**, pp. 879-892, 2021.
5. H.G. Krojanski and D. Suter. "Scaling of decoherence in wide NMR quantum registers". Phys. Rev. Lett. **93**, 090501, 2004.