Multiple-quantum NMR spectral intensity profiles under decoherence effects

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Multiple quantum (MQ) NMR spectroscopy of solids makes it possible not only to observe the growth and degradation of clusters of dynamically correlated spins, but also to control these processes using a controlled perturbation [1, 2]. The observed MQ spectrum is the sum of the MQ spectra from clusters with different numbers of spins K [3, 4] formed in a preparatory period of duration T. The contribution to above sum from different clusters of K spins we represented by a Gaussian MQ spectrum with a dispersion of $K/2$ multiplied by the weight function [3, 4] and by the function $\exp(-KB^2\tau^2/2)\exp(-A^2M^2\tau^2)$ what describes the cluster degradation [4]. The parameter B^2 characterizes the uncorrelated contribution to the local dipole field at the every spin of a cluster, and it does not depend on the local field at others spins, while parameter A^2 characterizes the field averaged over the cluster, and it acts in a correlated manner on all spins of the cluster. M is the coherence order. According the scheme of the experiment [1], $\tau = t_1$ is the duration of the evolution interval located between the preparatory interval and the mixing one, while with the scheme [2], $\tau = pt_T$, where t_T is the average time of occurrence of coherence on the interval $[0, T]$ [4], p is a small parameter. We have calculated the observed MQ spectrum numerically, and also obtained a simple formula for it by the saddle-point method:

$$G_M(T,\tau) \sim \exp\left\{-2\sqrt{2M^2\left(1+\bar{K}_0B^2\tau^2/4\right)\big/\bar{K}_0} - A^2M^2\tau^2\right\} ,$$

where $\bar{K}_0 = 1 + 2sh^2(T/\sqrt{2})$.

The formula obtained qualitatively correctly describes the results of calculations of the MQ spectra and experimental facts: the transformation of the Gaussian profile into an exponential one, the dependence of the relaxation rate of the MQ spectrum on M [1], and also the narrowing and stabilization of the MQ spectrum under the action of a perturbation [2].

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