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Simulations of quantum spin decoherence and spin diffusion using coherent-state representation[1] VIATCHESLAV DOBROVITSKI, Ames Laboratory US DOE, Iowa State University, Ames, IA, 50011 — Understanding non-equilibrium spin dynamics and spin diffusion in open quantum systems is of fundamental importance. It is also essential e.g. for NMR characterization of materials based on the spin diffusion between different ^{13}C sites. However, exact numerical modeling of large 3-D spin systems with arbitrary-range couplings is exponentially difficult, and approximate methods for such systems are actively sought. We consider the approach based on the coherent-state P-representation for the density matrix of the many-spin system [1], as applied to spin decoherence and spin diffusion in the presence of the spin bath. We consider both model spin systems (such as the central spin problem), and realistic NMR experiments (spin diffusion in graphite bilayers and in organic molecular crystals). The approximate modeling results are compared with the exact simulations performed on the systems of 20-25 spins. We determine the features of the system which justify the use of the P-representation modeling, and demonstrate that this approach is applicable to a wide range of situations important for quantum information processing and NMR experiments.
[1]K. Al-Hassanieh et al., Phys. Rev. Lett. 97, 037204 (2006); V. V. Dobrovitski et al., Phys. Rev. Lett. 102, 23760 (2009)

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