Two-spin and multi-spin quantum entanglement in V12 polyoxovanadate molecular nanomagnet

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Molecular nanomagnets constitute a highly interesting class of modern magnetic materials and offer a plethora of intriguing properties of quantum origin [1]. One of the possible applications of such systems can be connected with quantum computations [2-4]. For implementing the quantum algorithms, the presence and sufficient persistence of quantum entanglement is at least a desirable feature.

In the paper we present the computational study of quantum entanglement in V12 polyoxovanadate molecular cluster nanomagnet [5]. Its low-temperature magnetic properties are ruled by the behaviour of the non-interacting tetramers composed of quantum spins $S = 1/2$ [5,6]. The theoretical characterization of the system of interest is based on anisotropic quantum Heisenberg model. Both spin-space anisotropy and anisotropy related to the presence of two unequal couplings in the tetramer are included. The thermodynamic description is constructed using canonical ensemble in the presence of the external magnetic field. The exact analytic and numerical diagonalization is applied to the Hamiltonian; the interaction parameters are taken from the experiment [5].

The most typical two-particle entanglement is quantified using the Wootters concurrence [7], measuring the entanglement of formation. The values of Wootters concurrence are investigated for V12 as a function of the temperature and the external magnetic field, using analytic and numerical approach. The importance of the anisotropies in the studied tetramer for the quantitative description of the quantum entanglement is emphasized. To supplement the results concerning the two-particle entanglement and to capture a broader category of multiparticle entanglement, the fidelity [8] is used and its behaviour is discussed. The effect of quantum level crossings present in the energy spectrum of V12 on the studied properties is highlighted.

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