Quantum Entanglement Generation in Heterometallic $Ni^{2+}_4Gd^{3+}_4$ Complexes

Azam Zoshki[1],
Hamid Arian Zad[1], Michal Jaščur[1], Ralph Kenna[2], and Nerses Ananikian[3]
[1]*Department of Theoretical Physics and Astrophysics, Faculty of Science, P. J. Šafárik University, Park Angelinum 9, 041 54 Košice, Slovak Republic.*
[2]Centre for Fluid and Complex Systems, Coventry University, Coventry CV1 5FB, UK.
[3]A. I. Alikhanyan National Science Laboratory, 0036 Yerevan, Armenia.
zoshkia@yahoo.com

Molecular magnets with interacting spins [1] provide a powerful platform for advancing quantum science and technology. Their complex low-energy spectra make them promising candidates for quantum information storage and processing. We investigate various types of quantum entanglement [2] in the octanuclear heterometallic 3d/4f complexes denoted as $Ni^{2+}_4Gd^{3+}_4$ under an external magnetic field, using the exact diagonalization approach. These molecular magnets, which can be effectively described by Heisenberg spin models, consist of two identical $\{Ni^{2+}_2Gd^{3+}_2\}$ cubane subunits bridged by acetate and hydroxide ligands. Our analysis reveals that their magnetization exhibits intermediate plateaus at low temperatures, indicating distinct ground states characteristic of Ni-containing compounds. Using negativity as a measure of quantum entanglement, we examine the influence of single-ion anisotropy and magnetic field on tetrapartite, bipartite, 1–3 tangle, and 2–2 tangle entanglements in two families of $Ni^{2+}_4Gd^{3+}_4$ complexes: (1) without anisotropy [3] and (2) with anisotropy [4]. Complex (1) exhibits strong bipartite entanglement between Ni ions, which persists up to T ≈ 3.0K and B ≈ 4.0T, but shows significantly weaker tetrapartite entanglement and vanishing bipartite entanglement between Gd⋯Gd and Ni⋯Gd pairs. In contrast, complex (2) displays nonzero and sizable values for all types of entanglement considered. These findings emphasize the crucial role of single-ion anisotropy in generating and shaping the entanglement landscape of heterometallic $Ni^{2+}_4Gd^{3+}_4$ complexes. Notably, we find that the 1–3 tangle entanglement between a Ni ion and the remaining sites in a cubane unit serves as a reliable indicator of ground-state phase transitions, exhibiting distinct changes across phase boundaries irrespective of the presence of single-ion anisotropy.

Acknowledgments: A. Zoshki acknowledges the financial support provided by the EU NextGenerationEU through the Recovery and Resilience Plan for Slovakia under the project Nos. 09I03-03-V04-00403 and 09I03-03-V05 00008 (VVGS-2023-2888).

References

[1] O. Kahn, Molecular Magnetism, Wiley-VCH, 1993.
[2] R. Horodecki *et al*., Rev. Mod. Phys., 81, (2009) 865.
[3] M. Biswas, E. C. Sañudo, and D. Ray, Chem. Asian J. 15, (2020) 2731.
[4] P. Kalita, J. Goura, J. M. Herrera, E. Colacio, and V. Chandrasekhar, ACS Omega 3, (2018) 5202.

Figures

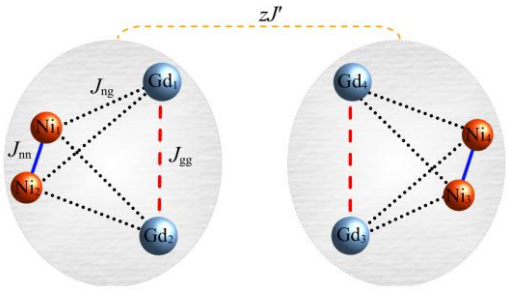

Figure 1: Schematic representation of the molecular structure of Ni^{2+}_4 Gd^{3+}_4 complexes.