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Exact and quasi exact numerical methods for giant magnetic molecules JÜRGEN SCHNACK, University of Bielefeld, Germany — The determination of the energy spectra of large magnetic molecules is a demanding numerical problem. In this contribution we demonstrate that theory has advanced very much in recent years. We first show that it is possible to diagonalize the Heisenberg Hamiltonian by employing the spin-rotational symmetry SU(2) in combination with arbitrary point-group symmetries [1]. This goes far beyond earlier approaches and enables us to evaluate thermodynamic observables such as the magnetization and spectroscopic data for molecules as large as the famous ferric wheel Fe_{10} with a Hilbert space dimension of more than 60 Millions. Then we explain how the finite-temperature Lanczos method can be applied to magnetic molecules in order to determine thermodynamic functions for Hilbert spaces as large as up to 1 Billion [2]. The new method enables us to discuss the magnetic properties of the highly frustrated Keplerate molecule $\{W_{72}V_{30}\}$ which behaves like a finite size Kagome lattice antiferromagnet.

[1] R. Schnalle and J. Schnack, Int. Rev. Phys. Chem. 29 (2010) 403; R. Schnalle, J. Schnack, Phys. Rev. B 79 (2009) 104419.
[2] J. Schnack, O. Wendland, Eur. Phys. J. B 78 (2010) 535-541.

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