Erratum: Thermodynamic observables of Mn_{12}-acetate calculated for the full spin Hamiltonian [Phys. Rev. B 92, 064424 (2015)]

Dennis Westerbeck, Oliver Hanebaum, and Jürgen Schnack

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The many variants to write down the Heisenberg spin Hamiltonian $\underset{\sim}{H} = \alpha \sum_{i<j} J_{ij} \underset{\sim}{\vec{s}}_i \cdot \underset{\sim}{\vec{s}}_j$ using as prefactors $\alpha = -1,\ +1,\ -2,\ +2$, or even $\pm 1/2$ in combination with the summation conventions $\sum_{i<j}$ or $\sum_{i,j}$ not only generates confusion, which sign addresses a ferromagnetic or an antiferromagnetic exchange interaction, it also leads to misunderstandings and misinterpretations of calculated exchange constants J_{ij}. Here, we report an error made in our earlier paper when using the model parameters for Mn_{12}-acetate obtained via density functional theory (DFT) in Ref. [1]. We erroneously assumed that the exchange constants given in Ref. [1] belong to a "$+J$"-Hamiltonian and, therefore, used values half as large as necessary. All other parameters of the full anisotropic Hamiltonian were not affected by the error.

The calculated effective magnetic moment as function of temperature is strongly affected by a factor of 2 in the J values since these are the largest contributions to the Hamiltonian. Therefore, one can estimate that features of the curve move to approximately twice the original temperature, compare Fig. 1 (right-hand side).

Our error was discovered in Ref. [5] and thankfully communicated to us by R. Sessoli. It was later confirmed by V. Mazurenko, one of the authors of Ref. [1]. We redid the full calculation with an independent new finite-temperature Lanczos code based on Ref. [6]. Meanwhile, science has progressed, and alternative approaches are available to address the spin Hamiltonian of Mn_{12}-acetate, see, e.g., Refs. [7,8].

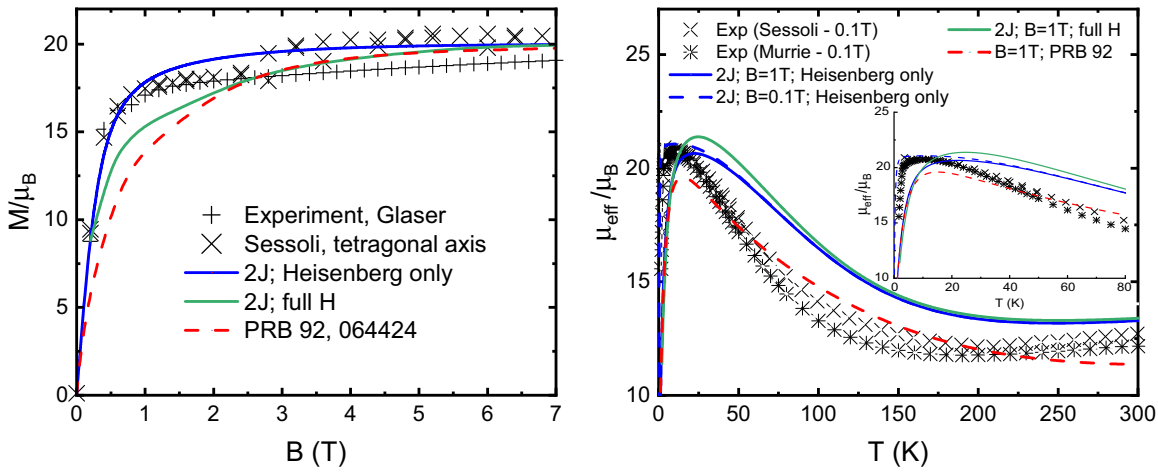

FIG. 1. Magnetization at 2 K and effective magnetic moment of Mn_{12}-acetate. The green and blue curves show the calculation with the corrected Heisenberg interactions from Ref. [1], whereas, the red ones are those from our paper. The powder average is performed over a regular grid of 10 directions on the unit sphere [2]. Data of Sessoli [3] and Murrie [4] are given by symbols.

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