Influence of Magnetic Field Averaging on Modeling Magnetic Properties of Molecular Nanomagnets

M. Antkowiak[1,2]

[1] *Faculty of Physics and Astronomy, Adam Mickiewicz University, ul. Uniwersytetu Poznańskiego 2, 61-614 Poznań, Poland*

[2] *Departament de Química Inorgànica i Orgànica, Universitat de Barcelona, Diagonal 645, 08028 Barcelona, Catalonia, Spain*

Accurate modeling of the magnetic properties of powder samples, particularly molecular nanomagnets, requires careful consideration of magnetic field averaging due to the random orientation of the applied field relative to individual crystallites. In this study, we employ the exact diagonalization method to compute key magnetic properties, such as magnetization and magnetic susceptibility, under different field averaging schemes. We investigate the validity of commonly used approximations and compare them with more sophisticated averaging methods. Our results demonstrate that for spin s=1, the conventional averaging approach – where only the z and x directions of the applied magnetic field are considered, with weights of $\frac{1}{3}$ and $\frac{2}{3}$, respectively – yields results nearly identical to those obtained through more detailed averaging techniques. However, for larger spin values, the choice of averaging method becomes increasingly critical, as improper field averaging can lead to significant deviations in calculated magnetic properties.

Additionally, we explore the role of magnetic anisotropy in influencing the powder-averaged magnetization and susceptibility, highlighting cases where strong anisotropy leads to noticeable deviations from isotropic expectations. To improve the accuracy of our modeling, we analyze the proper distribution of points on a sphere for orientational averaging, following established mathematical approaches while considering the symmetry between the x and y directions. Unlike Monte Carlo-based methods, which rely on stochastic sampling, our approach ensures systematic and reproducible results by employing well-defined sphere point distributions.

Our findings emphasize the necessity of selecting an appropriate averaging scheme when modeling powder samples, particularly for systems with high spin or pronounced anisotropy. The insights gained from this study contribute to the refinement of theoretical models and provide guidance for interpreting experimental data on molecular nanomagnets.