

Jiaming Wang

McMaster University

Nuclear Quadrupole Resonance Frequency of Cu in Herbertsmithite Kagome Heisenberg Antiferromagnet

Abstract:

An important property of the Cu in Herbertsmithite is its nuclear quadrupole resonance frequency ν_Q . The atom's electric quadrupole moment interacts with the electric field gradient (EFG) exerted on it by ionic and lattice charges [2] [3]. In order to approximate the EFG exerted on the Cu atoms. A static, classical model of the Herbertsmithite lattice was simulated using Python by approximating each ion as a point charge. ν_Q can also be measured experimentally using a technique related to Nuclear Magnetic Resonance known as Nuclear Quadrupole Resonance (NQR). This was done on Cu in Herbertsmithite by Imai et. al. [6]. The NQR experimental values of ν_Q (40.6MHz and 37.4MHz for ^{63}Cu and ^{65}Cu respectively) were in agreement with the lattice simulation results ($40.4 \pm 2\text{MHz}$ and $37.4 \pm 2\text{MHz}$).

References:

- [1] Zeeya Merali, *New Scientist* (2007).
- [2] C. P. Slichter, *Harper & Row* (1963).
- [3] A. Abragam, *Oxford University Press* (1961).
- [4] T. Shimizu, *J. Phys. Soc. Jpn.* **62**, 2, 779-784 (1993).
- [5] G. H. Fuller, *J. Phys. Chem. Ref. Data* **5**, 835 (1976).
- [6] T. Imai, E. A. Nytko, B. M. Barlett, M. P. Shores, and D. G. Nocera. *Phys. Rev. Lett.* **100**, 077203 (2008).