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Data analysis for µSR experiments with negative muons.

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Negative muons are often overlooked compared to their positive counterpart, partly due to the loss of around $\frac{5}{6}$ of the μ^- spin polarisation when a μ^- cascades down to the 1s muonic ground state after being captured by a nucleus. One needs to count for around 36 times as long to get statistics comparable to that of a μ^+SR experiment. However, there has been a recent revival of μ^-SR experiments, particularly in the study of hydrogen storage and battery materials [1,2]. When stopped in a material of atomic number Z, μ^- forms a muonic atom and cascades down to its ground state. The muon Bohr radius is 200 times smaller than the electron Bohr radius, and so this probe behaves like an ultra-dilute atom of apparent nuclear charge $Z - 1$. The μ^- will be strongly hyperfine coupled to the nuclear spin of the capture atom, but if that nuclear spin is zero, such as an oxygen in MnO, the only coupling will be to the nuclear dipolar fields in a region very close to that capture nucleus. Because of these difficulties new analysis techniques have been developed in WiMDA [3] for the fitting of μ^-SR data, and we have adapted the DFT+μ^+ technique for the case of a negative muon. Both of these new techniques have been applied to MnO where the dipole field simulations show a large field at the oxygen site, and DFT+μ^- calculations show a Jahn-Teller-like distortion around the negative muon.

References

[1] J.Sugiyama *et al* Phys. Rev. Lett. 121, 087202 (2018).

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