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Extension of Dynamical Kubo-Toyabe Relaxation Function for Refinement of Ion Dynamics Analysis

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The dynamical Kubo-Toyabe (DKT) relaxation function predicts the time evolution of muon spin polarization under zero and low longitudinal magnetic fields, which is determined by the linewidth Δ due to the static distribution of the internal magnetic field $\mathbf{H}(t)$ and its fluctuation frequency ν. One of its important features is that it can clearly distinguish two causes of decreasing linewidth in transverse-field muon spin relaxation (TF-μSR) that are hardly discernible: changes in the static field distribution (e.g., due to muon site change) and that associated with ν (motional narrowing) [1]. This is a powerful feature in the study of muon diffusion in metals, and the decrease in the linewidth at low temperatures observed in TF-μSR experiments has been identified as an effect of fluctuations due to quantum diffusion of muons [2].

On the other hand, the success of the DKT function in muon diffusion studies has seemingly created the misconception that the DKT function has proven to be applicable regardless of the source of fluctuations in $\mathbf{H}(t)$. It must be stressed here that every phenomenology including the DKT model has preconditions with which it can be applied: the dynamical model underlying the DKT function requires that the autocorrelation $\langle\mathbf{H}(0)\mathbf{H}(t)\rangle$ is entirely lost as $\propto \exp(-\nu t)$. Noting that this condition is non-trivial for the muons subjected to the local dynamics of ions in solids which has been the focus of much research in recent years [3], we have extended the DKT model to the case where only a part of $\mathbf{H}(t)$ fluctuates [4,5]. In this presentation, we discuss how this new phenomenology provides not only a means for quantitative analysis based on the assumption of immobile muons, but also a way to evaluate the validity of this assumption. We may also refer to the similar extension of relaxation model for muonium and muonated radicals that allows discerning the causes of fluctuations for the hyperfine and/or nuclear hyperfine fields [6].

References

[1] R. S. Hayano, et al., Phys. Rev. B **20**, 850 (1979).
[2] C. W. Clawson et al., Phys. Rev. Lett. **51**, 114 (1983).
[3] See, for example, M. Månsson and J. Sugiyama, Phys. Scr. **88**, 068509 (2013).
[4] T. U. Ito and R. Kadono, J. Phys. Soc. Jpn **93**, 044602 (2024).
[5] Plugin software for musrfit is available; see https://github.com/tuito0/musrfit-dynGssEALF
[6] R. Kadono and T. U. Ito, arXiv:2410.23575.

Email

ryosuke.kadono@kek.jp

Funding Agency

Supervisors Name

Supervisors Email

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Primary authors: KADONO, Ryosuke (KEK); Dr ITO, Takashi U. (ASRC, JAEA)

Presenter: KADONO, Ryosuke (KEK)

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