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The Static Muon Spin Relaxation Function for Li Ions in Graphite

The Kubo-Toyabe (KT) function has long been a mainstay of studies of ionic diffusion in solids. Its usefulness has extended far beyond its expected range of applicability. One of the assumptions of the KT theory is that there is a Gaussian distribution of internal fields reflecting the contributions of a dense array of nuclear spins surrounding the muon site. In many cases this is clearly not a good approximation. One example is for muons implanted into graphite intercalated with Li. From DFT+μ calculations on C_6Li using the CASTEP code it can be inferred that the muons form a short 1.1 A bond with C and two Li sites are close to the muon at 2.0 A and 2.8 A. These two spins alone account for 90 % of the dipolar Δ^2 sum. Besides dipolar coupling, quadrupolar coupling is also very important for Li ions and has a significant effect on the relaxation function. The static ZF relaxation function has been calculated for the relaxed muon site in C_6Li including interaction with these two Li sites. In comparison with the KT function, the calculated static relaxation function shows a suppressed 1/3 tail that is reminiscent of the effect of slow dynamics on the KT function, even though the model here is entirely static. Thus, it can be seen that a small number of quadrupolar spins can mimic the effect of dynamics in a dense spin system, providing a warning to take care when aiming to extract information about slow dynamics from the muon spin relaxation in such systems.

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