The Caldeira-Leggett model in the NMR context

Hampus Karlsson[1], **Marco Cazzaniga, Michele Ceotto**[1]

[1]*Dipartimento di Chimica, Università degli Studi di Milano, via Golgi 19, 20133 Milano, Italy*

In this project, we explore different semiclassical methods, and how they can be applied to study the impact of a surrounding environment on nuclear spin relaxation and various nuclear magnetic resonance (NMR) phenomena. Of particular interest has been the application and adaption of the Caldeira-Leggett formalism [1], in order to simulate line broadening effects in NMR spectra. We do this by utilizing the ideas of Meyer & Miller [2] and others [3], by treating the real and complex parts of the complex coefficients associated with the quantum spin states as classical variables. This makes it easier to rationalize the coupling between the spin degree of freedom and the classical harmonic oscillators of the surrounding environment. On the contrary to how the Caldeira-Leggett formalism or the "Spin-Boson [4] model" is usually used, i.e. to model the impact of the environment on the transition and tunneling between discrete energy states, a large part of our adaptions for simulating line broadening effects instead focus on how it can be used to model dephasing of the coherence associated with an ensemble of spins. Our numerical simulation results, show how the model introduce a line broadening effect in simulated NMR spectra, and how broadening increases with longer correlation times of the surrounding environment, in line with existing relaxation theories of NMR. These are results that show promise, and with some further improvements and details worked out concerning thermodynamical properties of the oscillators of the environment, the methods can be useful alternatives for modeling relaxation within the field of NMR.

[1] Caldeira, A.O.; Leggett, A.J. Annals of physics. **149**, 374 (1983).
[2] Meyer, H.-D.; Miller, W.H. The Journal of Chemical Physics. **71**, 2156 (1979).
[3] Strocchi, F. Reviews of Modern Physics . **38**, 36 (1966).
[4] Leggett, A. J.; Chakravarty, S. *et al.* Reviews of Modern Physics. **59**, 1 (1987).